



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:08 PM BST

PDB ID : 1B8T
Title : SOLUTION STRUCTURE OF THE CHICKEN CRP1
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Deposited on : 1999-02-02

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
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

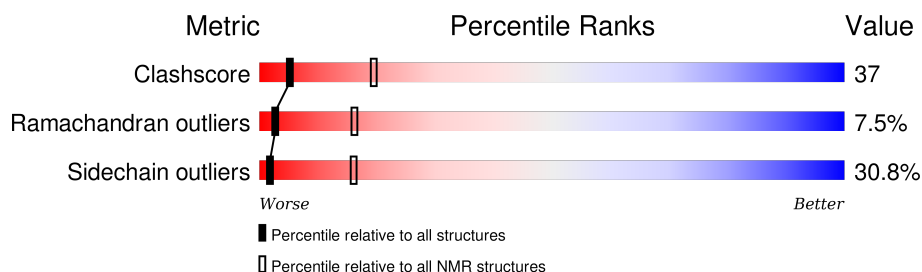
1 Overall quality at a glance

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	192	

2 Ensemble composition and analysis

This entry contains 37 models. Model 34 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:8-A:67 (60)	0.56	35
2	A:94-A:109 (16)	0.79	35
3	A:115-A:175 (61)	0.53	34

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, 6, 7, 8, 9, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 28, 29, 31, 34, 35, 37
2	23, 24, 26, 30, 32
3	10, 21, 33
4	22, 36
Single-model clusters	25; 27

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2773 atoms, of which 1356 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (CRP1).

Mol	Chain	Residues	Atoms						Trace
1	A	192	Total	C	H	N	O	S	0
			2769	876	1356	252	266	19	

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

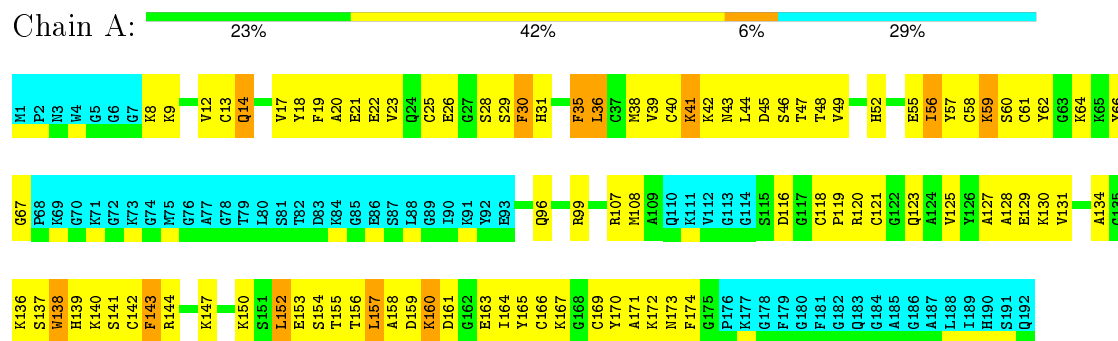
Mol	Chain	Residues	Atoms	
2	A	4	Total	Zn
			4	4

4 Residue-property plots [i](#)

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: PROTEIN (CRP1)

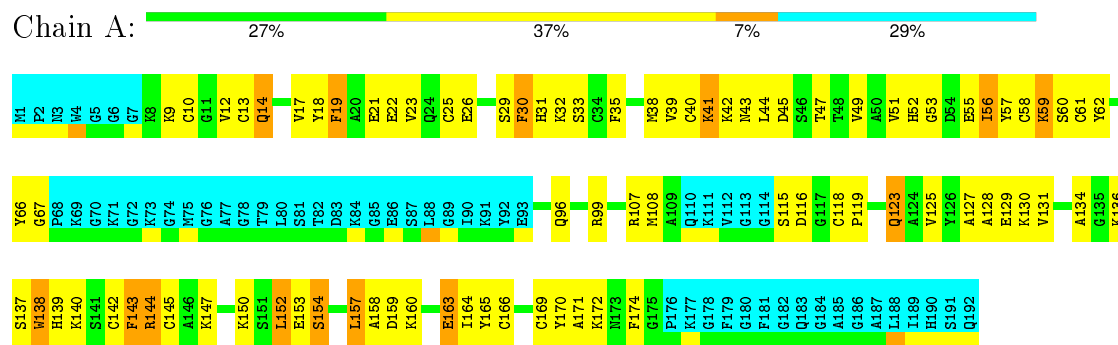


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

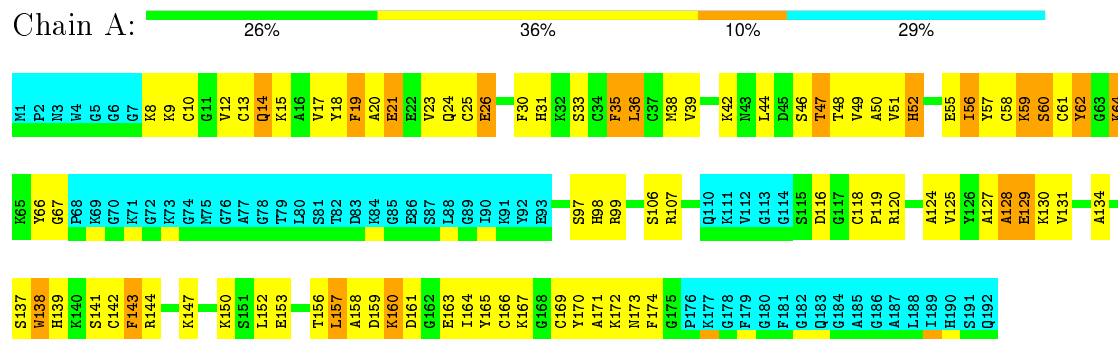
4.2.1 Score per residue for model 1

- Molecule 1: PROTEIN (CRP1)



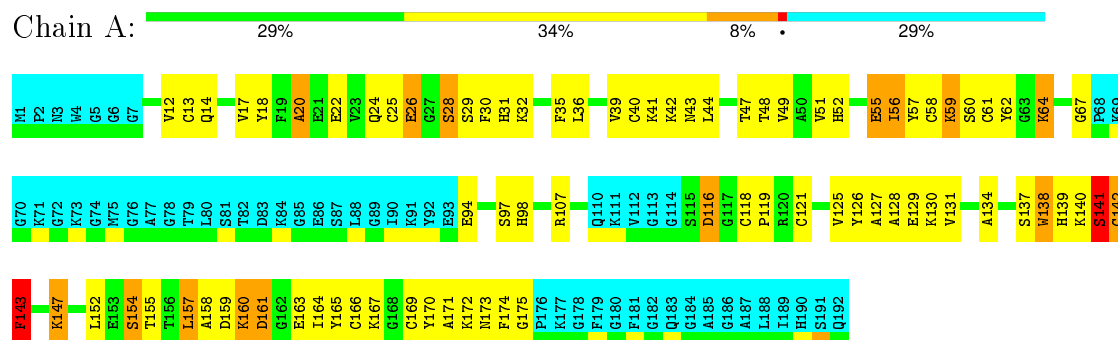
4.2.2 Score per residue for model 2

- Molecule 1: PROTEIN (CRP1)



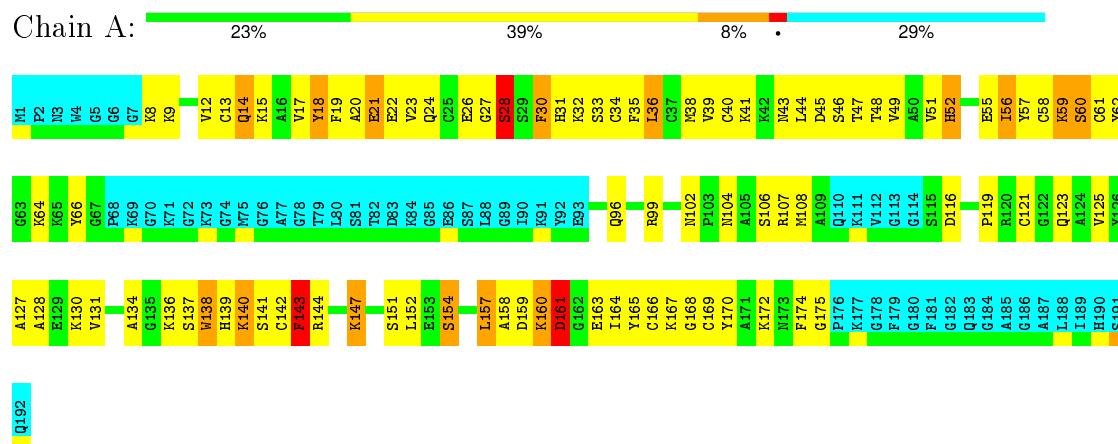
4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN (CRP1)



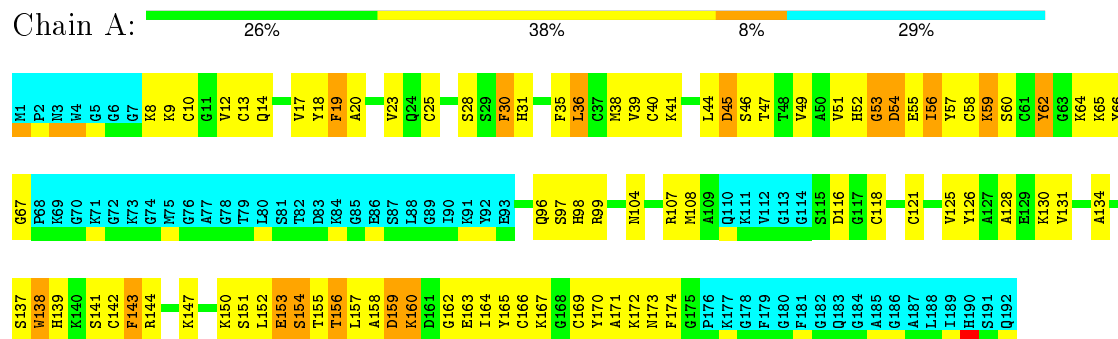
4.2.4 Score per residue for model 4

- Molecule 1: PROTEIN (CRP1)



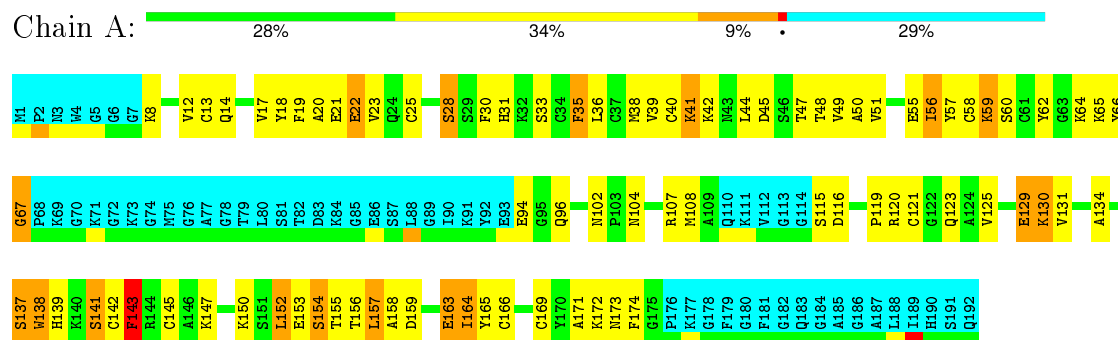
4.2.5 Score per residue for model 5

- Molecule 1: PROTEIN (CRP1)



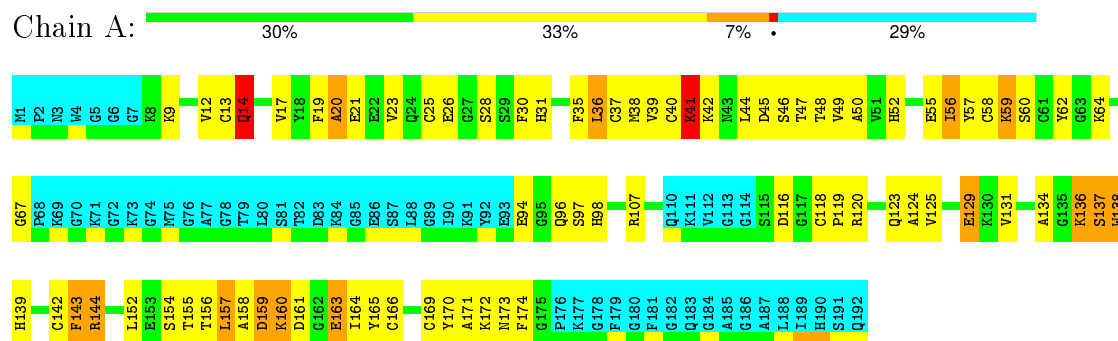
4.2.6 Score per residue for model 6

- Molecule 1: PROTEIN (CRP1)



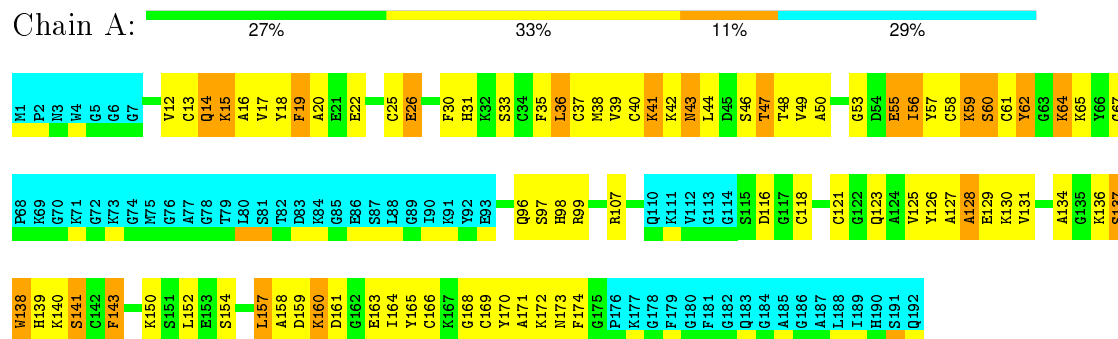
4.2.7 Score per residue for model 7

- Molecule 1: PROTEIN (CRP1)



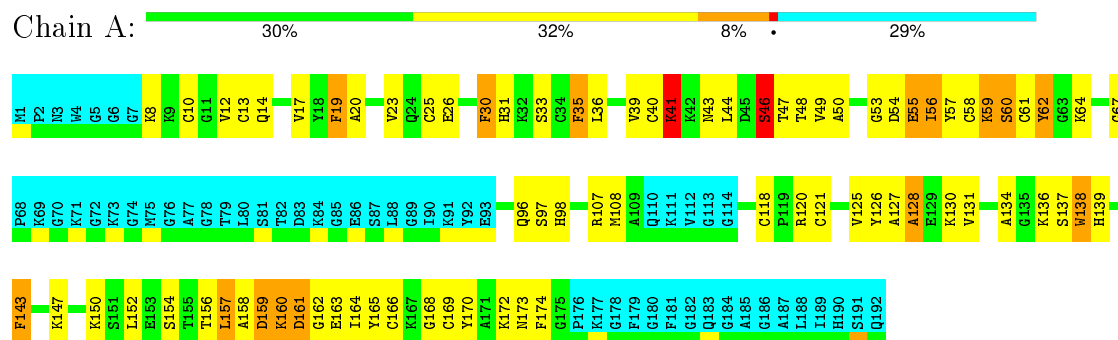
4.2.8 Score per residue for model 8

- Molecule 1: PROTEIN (CRP1)



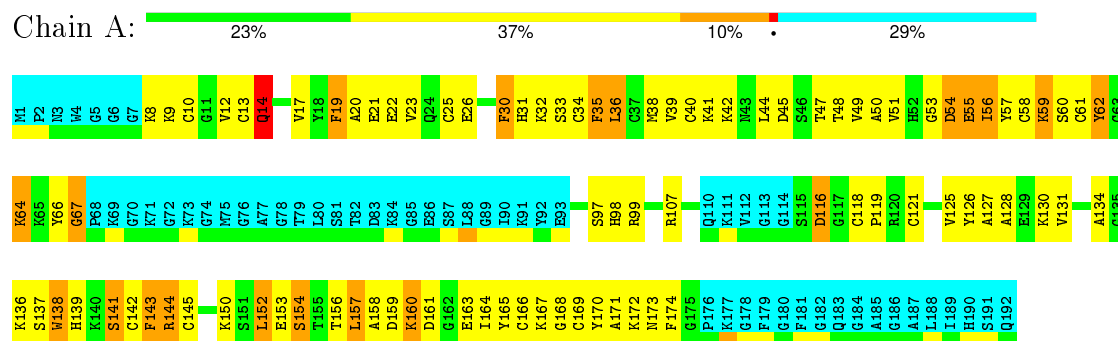
4.2.9 Score per residue for model 9

- Molecule 1: PROTEIN (CRP1)



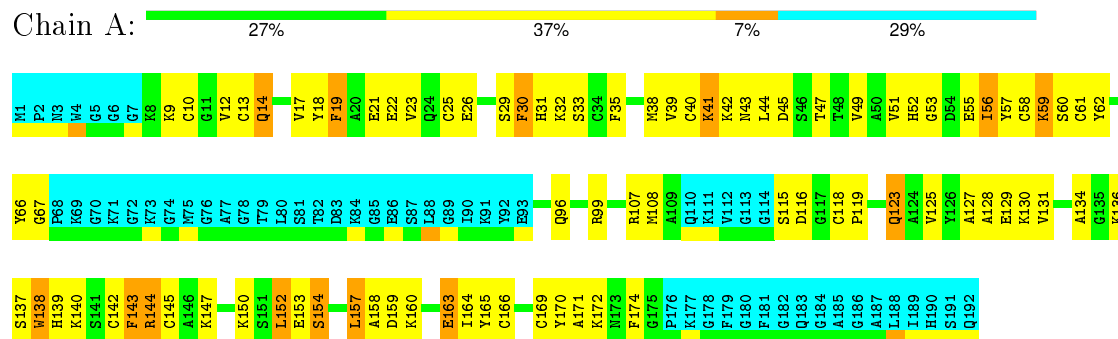
4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN (CRP1)



4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN (CRP1)



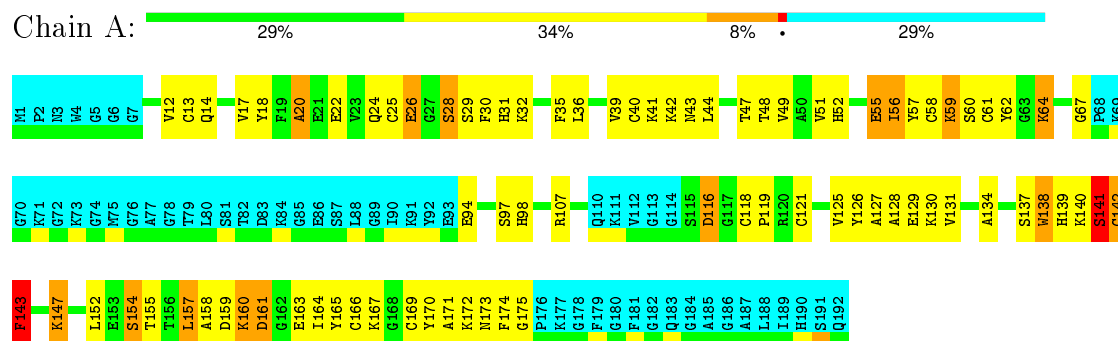
4.2.12 Score per residue for model 12

- Molecule 1: PROTEIN (CRP1)



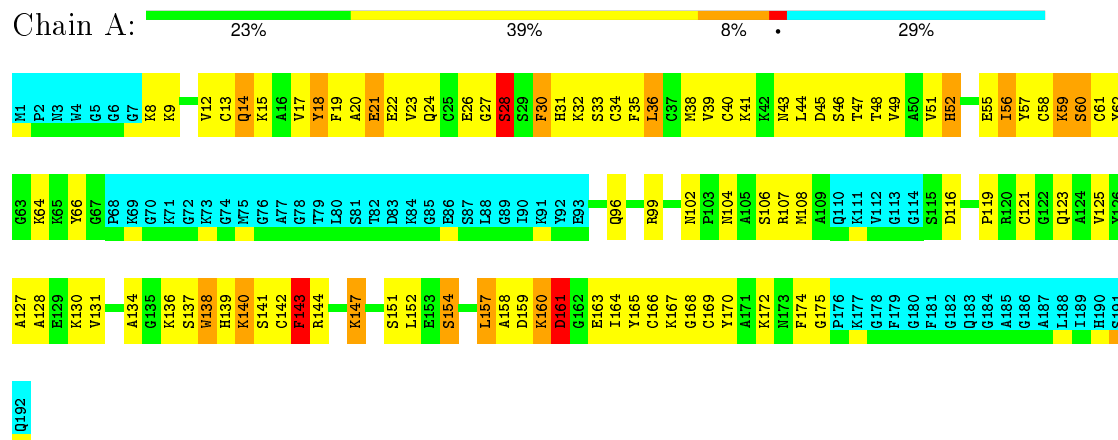
4.2.13 Score per residue for model 13

- Molecule 1: PROTEIN (CRP1)



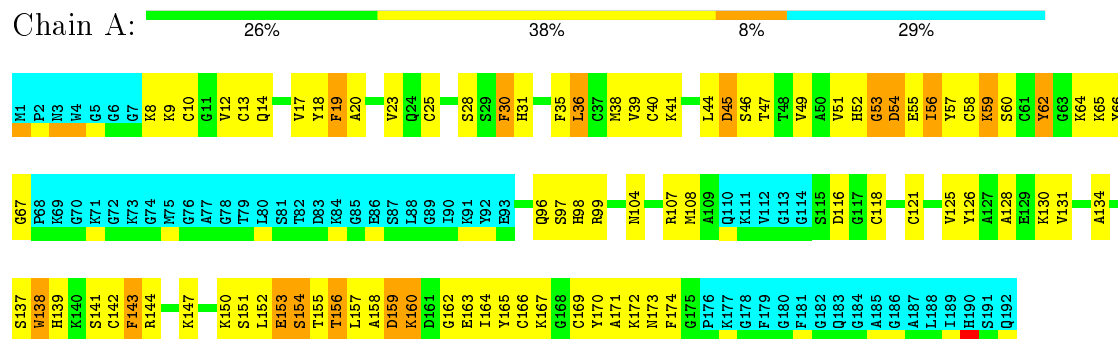
4.2.14 Score per residue for model 14

- Molecule 1: PROTEIN (CRP1)



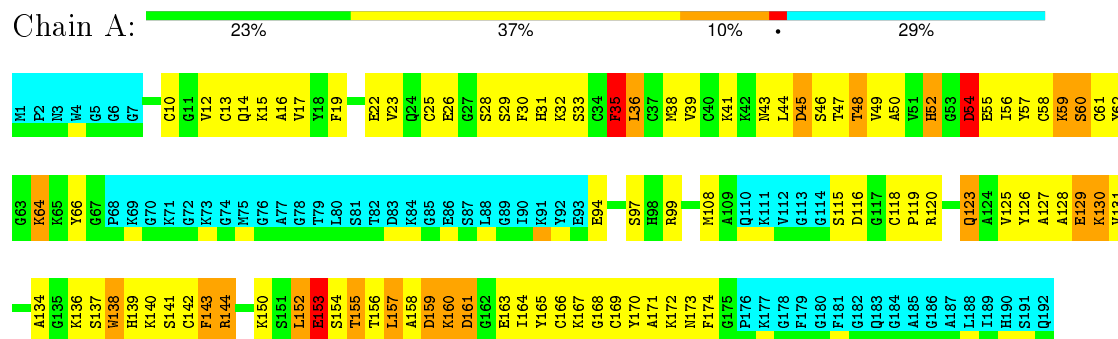
4.2.15 Score per residue for model 15

- Molecule 1: PROTEIN (CRP1)



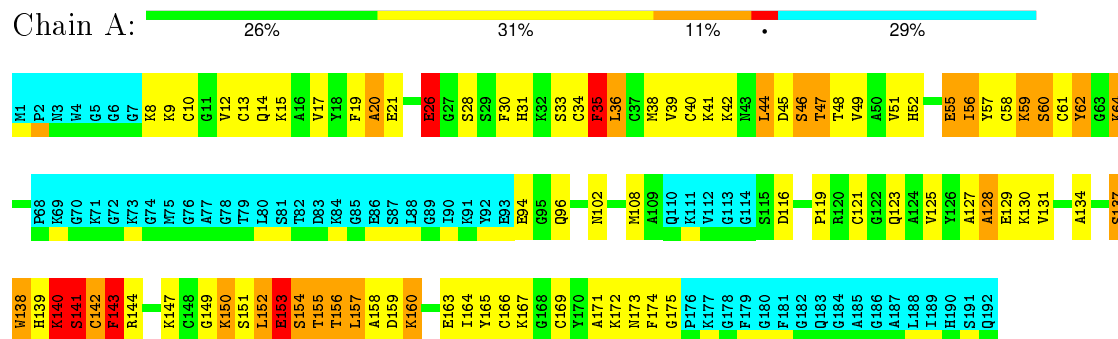
4.2.16 Score per residue for model 16

- Molecule 1: PROTEIN (CRP1)



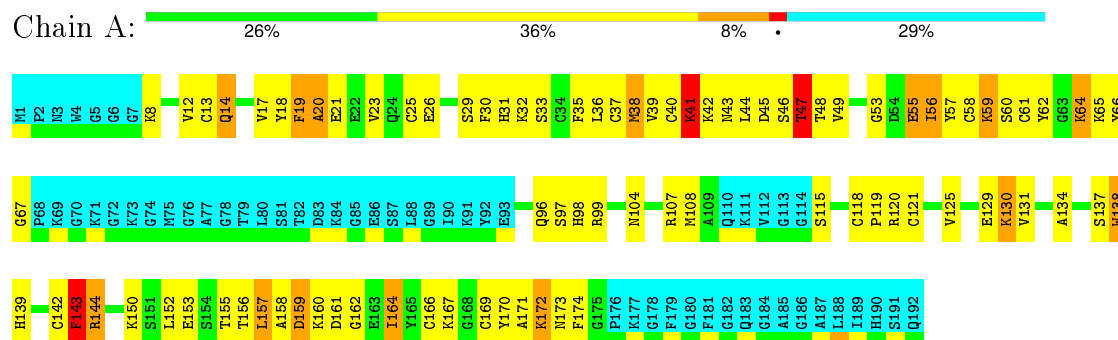
4.2.17 Score per residue for model 17

- Molecule 1: PROTEIN (CRP1)



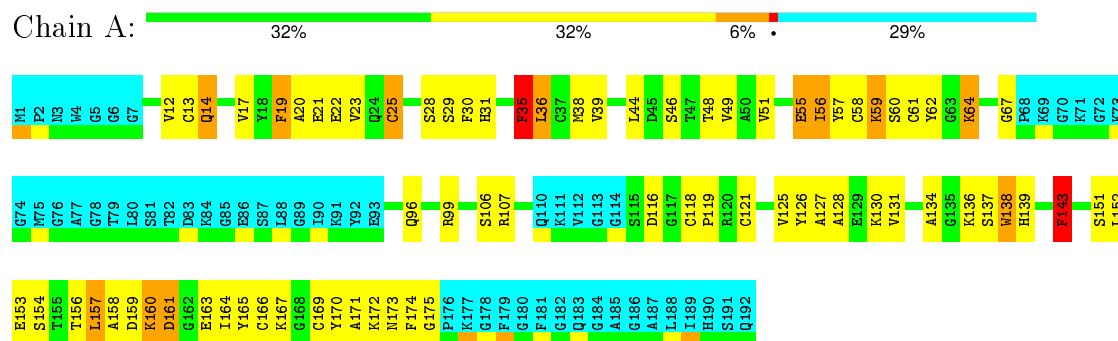
4.2.18 Score per residue for model 18

- Molecule 1: PROTEIN (CRP1)



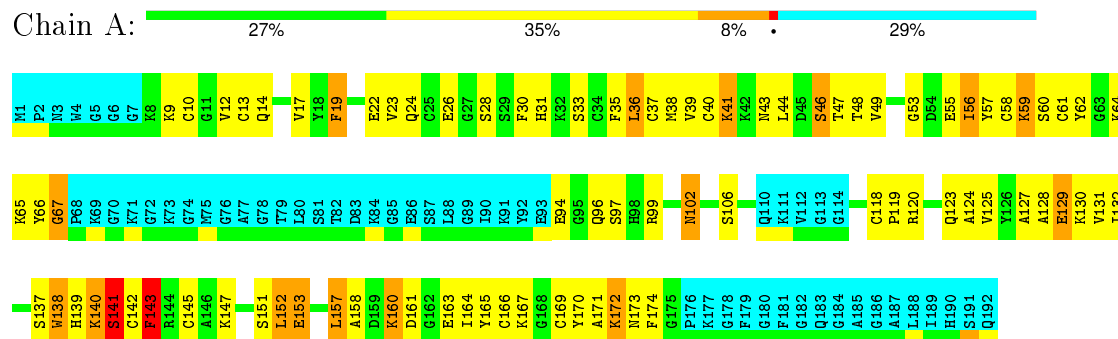
4.2.19 Score per residue for model 19

- Molecule 1: PROTEIN (CRP1)



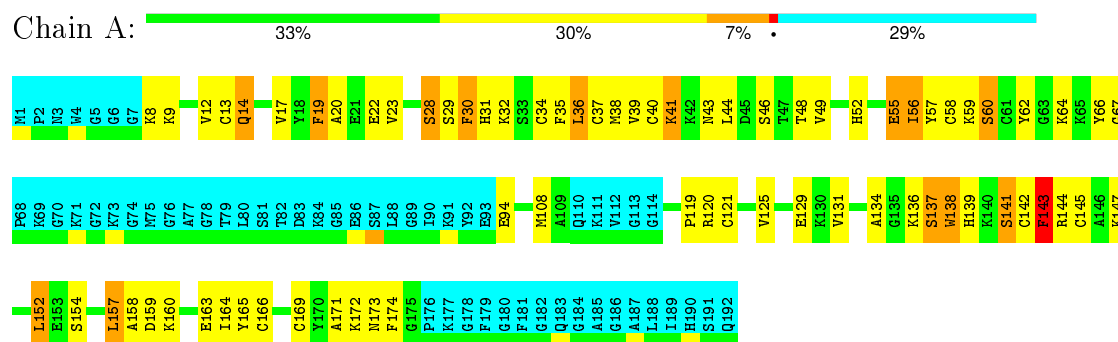
4.2.20 Score per residue for model 20

- Molecule 1: PROTEIN (CRP1)



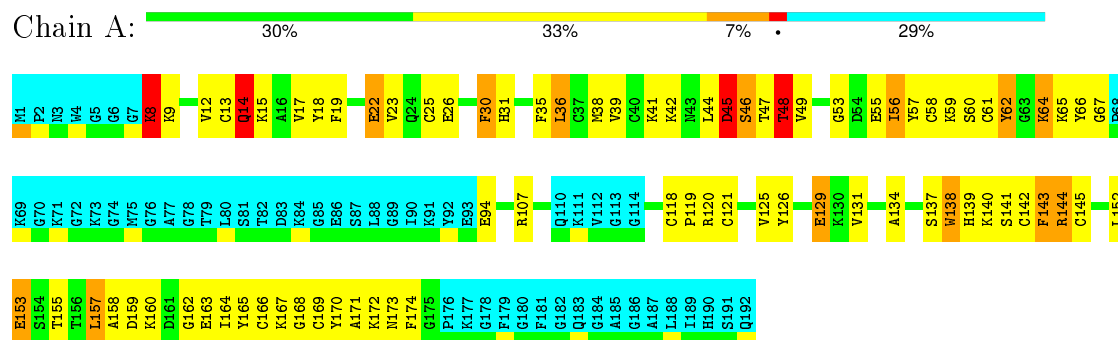
4.2.23 Score per residue for model 23

- Molecule 1: PROTEIN (CRP1)



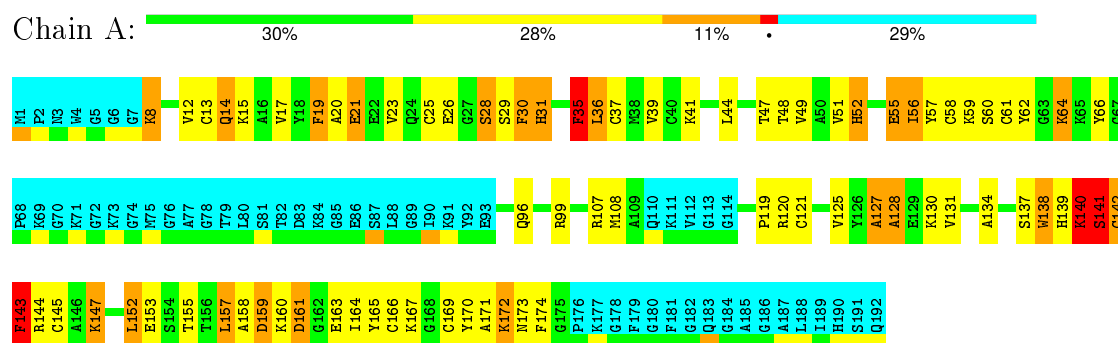
4.2.24 Score per residue for model 24

- Molecule 1: PROTEIN (CRP1)



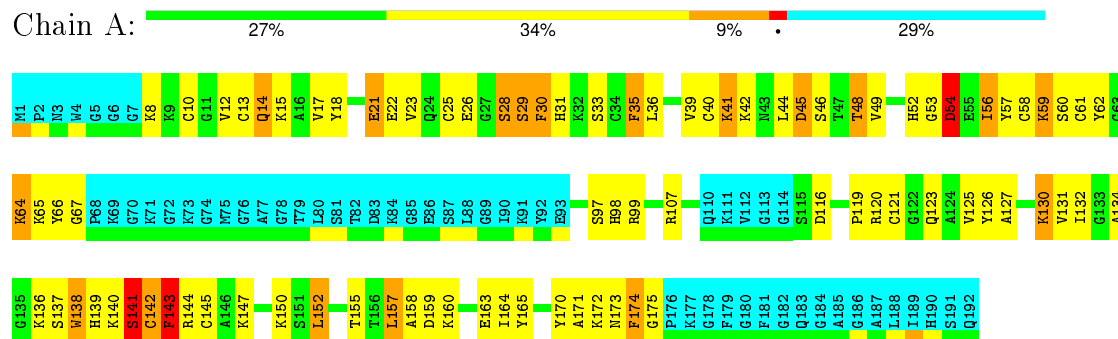
4.2.25 Score per residue for model 25

- Molecule 1: PROTEIN (CRP1)



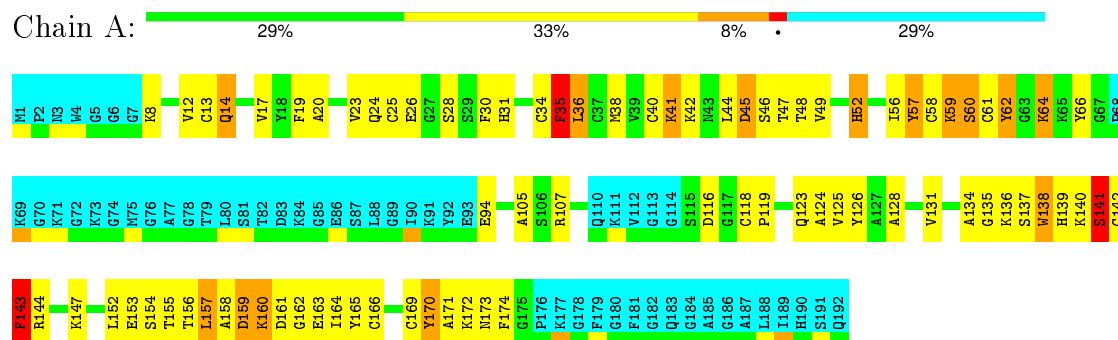
4.2.26 Score per residue for model 26

- Molecule 1: PROTEIN (CRP1)



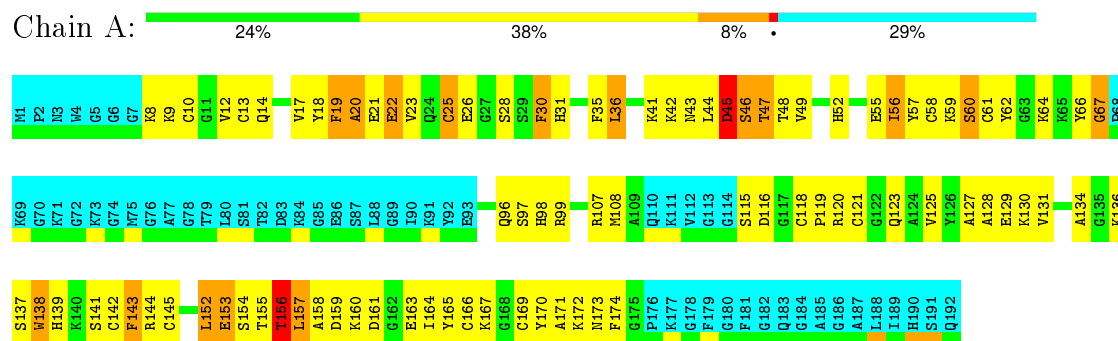
4.2.27 Score per residue for model 27

- Molecule 1: PROTEIN (CRP1)



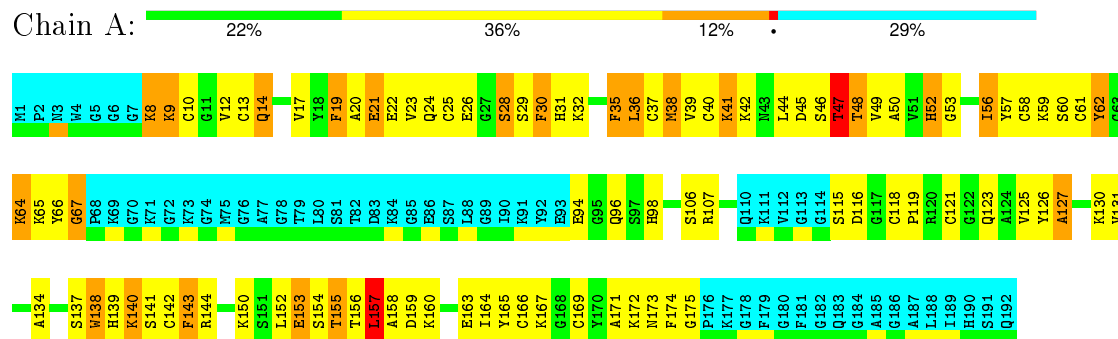
4.2.28 Score per residue for model 28

- Molecule 1: PROTEIN (CRP1)



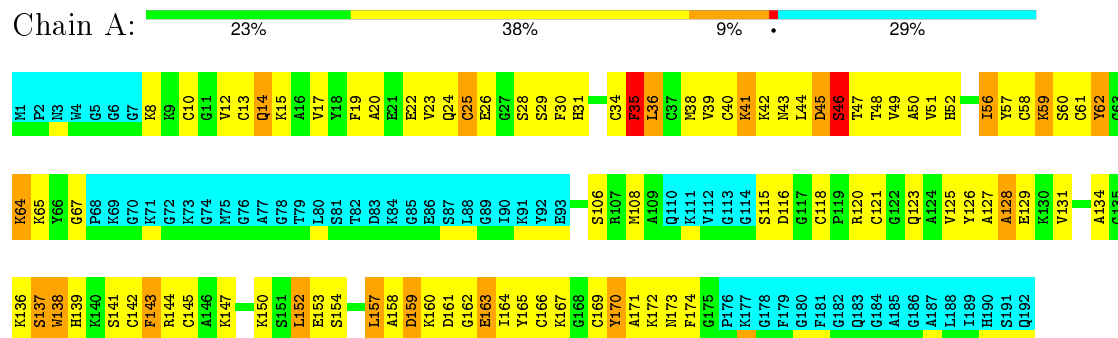
4.2.29 Score per residue for model 29

- Molecule 1: PROTEIN (CRP1)



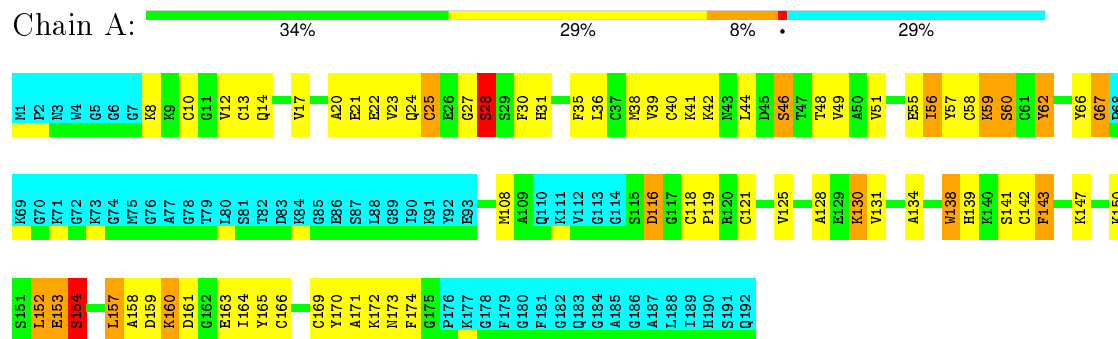
4.2.30 Score per residue for model 30

- Molecule 1: PROTEIN (CRP1)



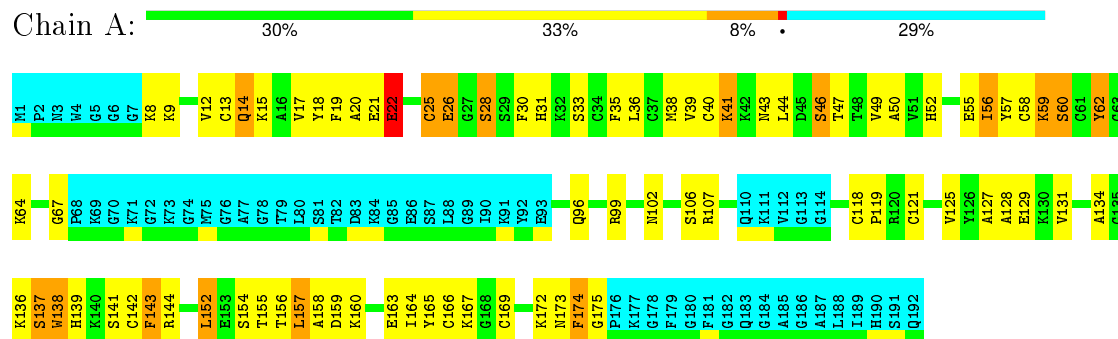
4.2.31 Score per residue for model 31

- Molecule 1: PROTEIN (CRP1)



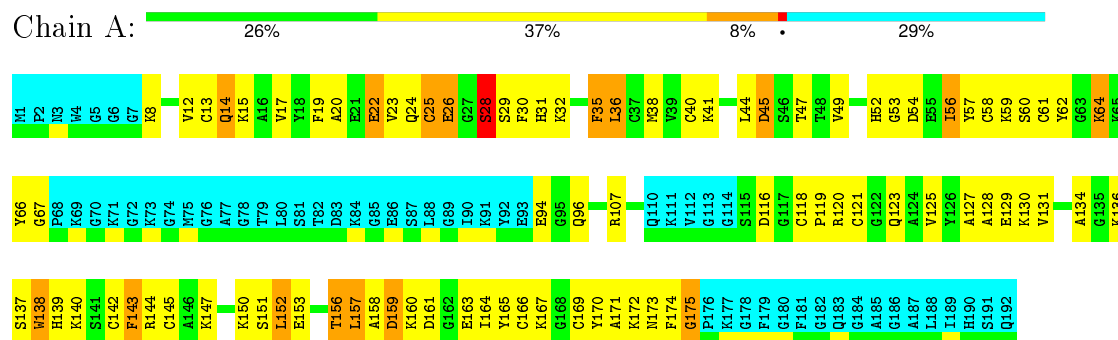
4.2.32 Score per residue for model 32

- Molecule 1: PROTEIN (CRP1)



4.2.33 Score per residue for model 33

- Molecule 1: PROTEIN (CRP1)



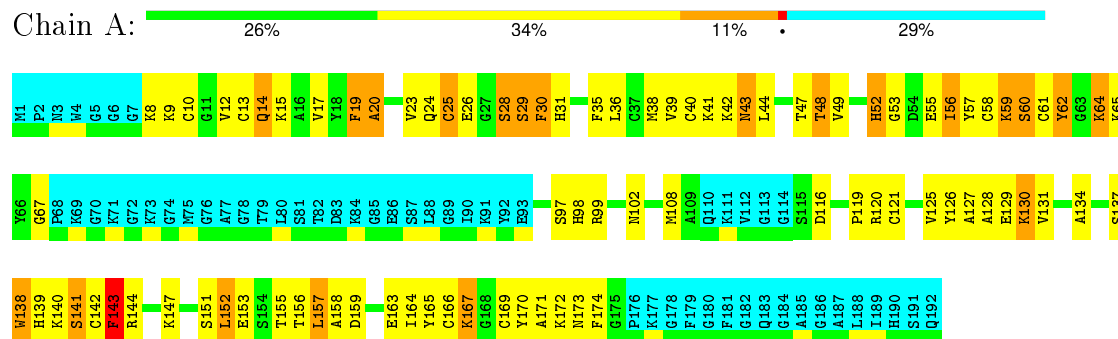
4.2.34 Score per residue for model 34 (medoid)

- Molecule 1: PROTEIN (CRP1)



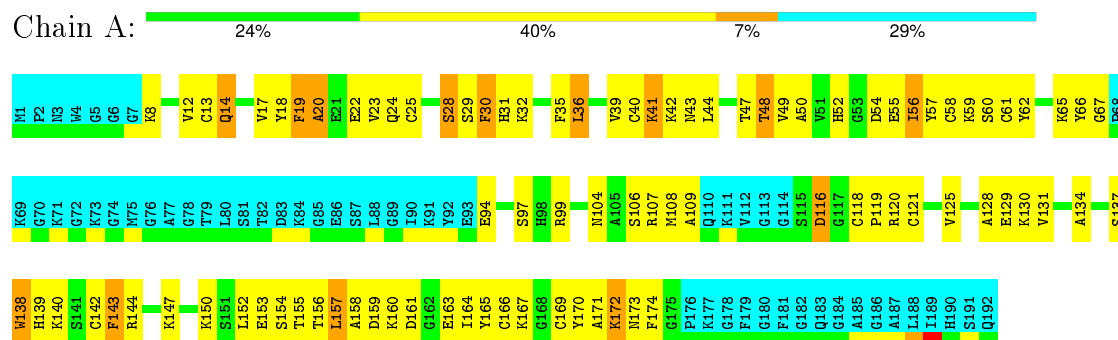
4.2.35 Score per residue for model 35

- Molecule 1: PROTEIN (CRP1)



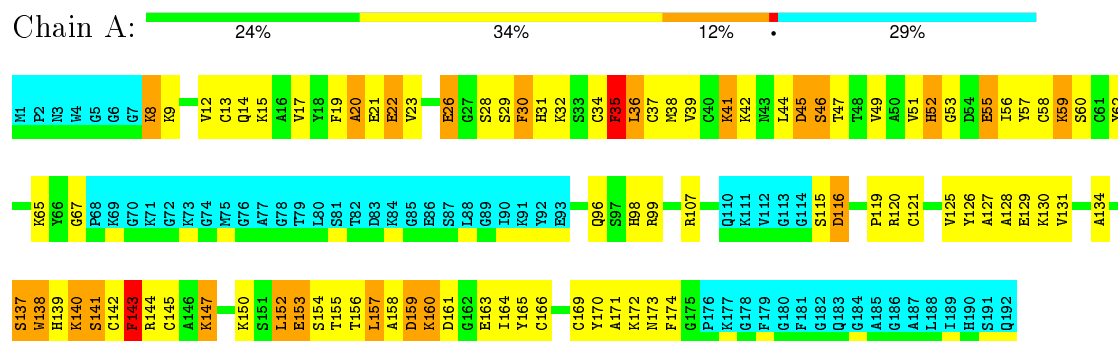
4.2.36 Score per residue for model 36

- Molecule 1: PROTEIN (CRP1)



4.2.37 Score per residue for model 37

- Molecule 1: PROTEIN (CRP1)



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DYANA*.

Of the 37 calculated structures, 37 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
DYANA	refinement	
NMRVIEW	structure solution	

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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	1032	981	989	75±8
All	All	38332	36297	36593	2766

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 37.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:PHE:CE1	1:A:164:ILE:HD13	1.06	1.86	7	35
1:A:50:ALA:HB3	1:A:62:TYR:CE2	0.98	1.94	6	5
1:A:17:VAL:HG22	1:A:31:HIS:NE2	0.98	1.74	25	37
1:A:39:VAL:HG23	1:A:57:TYR:CD1	0.96	1.95	18	32
1:A:157:LEU:HD12	1:A:158:ALA:N	0.94	1.78	28	36
1:A:17:VAL:HG22	1:A:31:HIS:CE1	0.94	1.97	22	34
1:A:131:VAL:HG12	1:A:138:TRP:O	0.93	1.64	14	37
1:A:44:LEU:HD13	1:A:49:VAL:HG23	0.92	1.39	28	20
1:A:44:LEU:HD22	1:A:49:VAL:HG23	0.90	1.40	6	6
1:A:35:PHE:CE1	1:A:49:VAL:HG21	0.86	2.06	8	36
1:A:125:VAL:HG22	1:A:139:HIS:CD2	0.85	2.06	21	36
1:A:44:LEU:HD21	1:A:58:CYS:HB3	0.82	1.51	23	29

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LEU:HD13	1:A:49:VAL:CG2	0.79	2.08	19	11
1:A:47:THR:HG22	1:A:48:THR:HG23	0.78	1.54	20	1
1:A:44:LEU:HD21	1:A:58:CYS:CB	0.78	2.09	26	19
1:A:143:PHE:CD1	1:A:164:ILE:HD13	0.78	2.12	6	30
1:A:12:VAL:HG23	1:A:30:PHE:CD1	0.77	2.15	31	35
1:A:155:THR:HG23	1:A:156:THR:HG23	0.76	1.54	16	1
1:A:23:VAL:HG11	1:A:35:PHE:CD2	0.76	2.16	16	23
1:A:17:VAL:HG22	1:A:31:HIS:CD2	0.76	2.16	17	31
1:A:145:CYS:HB2	1:A:152:LEU:HD21	0.74	1.60	26	13
1:A:131:VAL:HG12	1:A:138:TRP:C	0.74	2.02	19	17
1:A:125:VAL:HG22	1:A:139:HIS:NE2	0.74	1.96	8	36
1:A:35:PHE:CE1	1:A:56:ILE:HD11	0.74	2.17	16	1
1:A:36:LEU:HD11	1:A:41:LYS:O	0.74	1.83	28	13
1:A:36:LEU:N	1:A:56:ILE:HD11	0.74	1.98	23	15
1:A:39:VAL:CG2	1:A:57:TYR:CD1	0.72	2.72	26	32
1:A:62:TYR:CE2	1:A:66:TYR:CZ	0.72	2.78	33	5
1:A:48:THR:HG22	1:A:59:LYS:HB2	0.72	1.59	31	2
1:A:62:TYR:CE1	1:A:66:TYR:CZ	0.72	2.78	23	5
1:A:44:LEU:CD2	1:A:49:VAL:HG23	0.71	2.14	16	2
1:A:130:LYS:CE	1:A:132:ILE:HD11	0.70	2.16	20	1
1:A:143:PHE:CE2	1:A:157:LEU:CD2	0.70	2.74	25	12
1:A:44:LEU:HD12	1:A:56:ILE:CD1	0.70	2.17	33	3
1:A:50:ALA:CB	1:A:62:TYR:CE2	0.70	2.75	6	5
1:A:35:PHE:CD1	1:A:56:ILE:HD12	0.70	2.22	1	17
1:A:23:VAL:HG11	1:A:35:PHE:CD1	0.70	2.22	29	1
1:A:134:ALA:HB2	1:A:159:ASP:HB3	0.69	1.64	37	17
1:A:157:LEU:HD12	1:A:157:LEU:C	0.69	2.07	27	15
1:A:27:GLY:HA3	1:A:51:VAL:HG11	0.69	1.61	14	2
1:A:17:VAL:HG11	1:A:22:GLU:HG3	0.69	1.65	34	2
1:A:138:TRP:N	1:A:138:TRP:CD1	0.69	2.61	16	16
1:A:134:ALA:HB2	1:A:159:ASP:CB	0.69	2.18	35	28
1:A:138:TRP:CD1	1:A:138:TRP:N	0.69	2.61	18	21
1:A:50:ALA:HB3	1:A:62:TYR:CD2	0.68	2.22	36	5
1:A:62:TYR:CD1	1:A:66:TYR:CE2	0.68	2.81	5	2
1:A:35:PHE:CE1	1:A:56:ILE:HD12	0.68	2.22	1	10
1:A:19:PHE:O	1:A:19:PHE:CD2	0.68	2.46	24	5
1:A:156:THR:HG23	1:A:167:LYS:HD3	0.68	1.65	12	3
1:A:48:THR:HG22	1:A:59:LYS:CB	0.68	2.18	31	2
1:A:36:LEU:HD12	1:A:43:ASN:N	0.68	2.03	35	12
1:A:143:PHE:CE2	1:A:157:LEU:HD22	0.67	2.24	23	22
1:A:47:THR:HG23	1:A:48:THR:HG23	0.67	1.64	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:THR:O	1:A:47:THR:HG22	0.67	1.89	27	2
1:A:35:PHE:CD1	1:A:56:ILE:CD1	0.67	2.77	1	14
1:A:143:PHE:CE1	1:A:164:ILE:CD1	0.66	2.79	22	14
1:A:44:LEU:HD22	1:A:49:VAL:CG2	0.66	2.18	6	3
1:A:45:ASP:O	1:A:47:THR:HG23	0.66	1.90	33	1
1:A:143:PHE:CD1	1:A:164:ILE:CD1	0.66	2.79	34	15
1:A:143:PHE:CE1	1:A:164:ILE:HG21	0.66	2.26	23	5
1:A:52:HIS:CB	1:A:57:TYR:CE1	0.66	2.79	27	1
1:A:48:THR:O	1:A:48:THR:HG23	0.65	1.91	14	3
1:A:48:THR:HG23	1:A:48:THR:O	0.65	1.91	4	3
1:A:152:LEU:HD13	1:A:157:LEU:HB2	0.65	1.68	31	2
1:A:134:ALA:HB2	1:A:159:ASP:HB2	0.65	1.68	30	12
1:A:12:VAL:CG2	1:A:30:PHE:CD1	0.64	2.80	31	20
1:A:12:VAL:HG23	1:A:30:PHE:CE1	0.64	2.28	30	8
1:A:155:THR:HG23	1:A:156:THR:N	0.63	2.08	16	3
1:A:35:PHE:HE1	1:A:49:VAL:HG21	0.63	1.53	10	29
1:A:56:ILE:C	1:A:57:TYR:CD1	0.63	2.72	35	5
1:A:19:PHE:O	1:A:20:ALA:HB3	0.63	1.94	23	6
1:A:36:LEU:HD12	1:A:43:ASN:CA	0.62	2.24	14	10
1:A:137:SER:C	1:A:138:TRP:CD1	0.62	2.73	12	33
1:A:154:SER:HA	1:A:157:LEU:HD23	0.62	1.72	23	3
1:A:157:LEU:C	1:A:157:LEU:HD12	0.62	2.13	4	6
1:A:127:ALA:O	1:A:128:ALA:HB2	0.62	1.95	12	4
1:A:50:ALA:HB1	1:A:62:TYR:CE2	0.62	2.29	30	5
1:A:23:VAL:CG1	1:A:35:PHE:CD2	0.62	2.83	36	24
1:A:143:PHE:HE1	1:A:164:ILE:HD13	0.62	1.53	17	10
1:A:143:PHE:CE2	1:A:157:LEU:HD21	0.61	2.31	27	2
1:A:56:ILE:O	1:A:57:TYR:CD1	0.61	2.54	29	31
1:A:47:THR:HG23	1:A:48:THR:CG2	0.61	2.25	12	2
1:A:158:ALA:HB1	1:A:170:TYR:CD1	0.61	2.31	26	11
1:A:143:PHE:HE2	1:A:157:LEU:HD22	0.61	1.55	33	14
1:A:30:PHE:CE2	1:A:56:ILE:HG21	0.61	2.30	27	1
1:A:57:TYR:CD1	1:A:57:TYR:N	0.61	2.69	27	1
1:A:21:GLU:O	1:A:23:VAL:HG23	0.60	1.96	25	9
1:A:170:TYR:O	1:A:174:PHE:CD1	0.60	2.54	16	5
1:A:138:TRP:NE1	1:A:143:PHE:CZ	0.60	2.69	23	11
1:A:130:LYS:HD3	1:A:132:ILE:HD11	0.60	1.74	22	1
1:A:17:VAL:CG2	1:A:31:HIS:CE1	0.60	2.82	22	8
1:A:130:LYS:HE3	1:A:132:ILE:HD11	0.60	1.74	20	1
1:A:44:LEU:CD1	1:A:49:VAL:HG23	0.60	2.24	28	2
1:A:125:VAL:HG12	1:A:130:LYS:HG3	0.60	1.74	37	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:170:TYR:O	1:A:174:PHE:CD2	0.60	2.55	24	23
1:A:62:TYR:O	1:A:66:TYR:CD2	0.60	2.55	6	7
1:A:23:VAL:HG11	1:A:35:PHE:HD2	0.59	1.57	37	4
1:A:36:LEU:O	1:A:56:ILE:HD11	0.59	1.97	37	1
1:A:35:PHE:CZ	1:A:49:VAL:HG11	0.59	2.32	27	10
1:A:48:THR:O	1:A:48:THR:HG22	0.59	1.96	23	4
1:A:39:VAL:HG23	1:A:57:TYR:HD1	0.59	1.53	36	31
1:A:118:CYS:CB	1:A:139:HIS:CE1	0.59	2.85	19	25
1:A:157:LEU:HD12	1:A:158:ALA:O	0.58	1.98	13	15
1:A:12:VAL:HG12	1:A:13:CYS:N	0.58	2.13	10	32
1:A:156:THR:HG23	1:A:167:LYS:CD	0.58	2.28	12	3
1:A:12:VAL:HG11	1:A:34:CYS:HB3	0.58	1.76	10	5
1:A:62:TYR:CE1	1:A:66:TYR:OH	0.58	2.55	5	2
1:A:36:LEU:C	1:A:56:ILE:HD11	0.57	2.19	30	1
1:A:127:ALA:O	1:A:128:ALA:HB3	0.57	1.98	28	5
1:A:19:PHE:O	1:A:20:ALA:HB2	0.57	1.98	22	8
1:A:47:THR:O	1:A:48:THR:HG22	0.57	2.00	25	2
1:A:155:THR:O	1:A:156:THR:HG22	0.57	2.00	18	2
1:A:19:PHE:O	1:A:19:PHE:CG	0.57	2.57	24	1
1:A:37:CYS:HB2	1:A:44:LEU:HD11	0.56	1.77	29	5
1:A:57:TYR:N	1:A:57:TYR:CD1	0.56	2.73	34	4
1:A:52:HIS:CB	1:A:57:TYR:CE2	0.56	2.88	26	4
1:A:25:CYS:SG	1:A:35:PHE:CE2	0.56	2.99	6	5
1:A:18:TYR:CZ	1:A:20:ALA:CB	0.56	2.89	36	1
1:A:53:GLY:O	1:A:54:ASP:CB	0.56	2.53	5	2
1:A:50:ALA:HB3	1:A:62:TYR:CD1	0.56	2.36	34	1
1:A:18:TYR:CE1	1:A:19:PHE:CZ	0.56	2.94	34	1
1:A:138:TRP:CD1	1:A:143:PHE:CZ	0.56	2.93	21	5
1:A:28:SER:CB	1:A:30:PHE:CZ	0.56	2.89	17	3
1:A:140:LYS:O	1:A:141:SER:CB	0.56	2.54	13	8
1:A:173:ASN:CG	1:A:174:PHE:CE1	0.56	2.80	13	6
1:A:131:VAL:HG23	1:A:153:GLU:O	0.55	2.00	12	4
1:A:44:LEU:HD12	1:A:56:ILE:HD11	0.55	1.77	33	4
1:A:144:ARG:O	1:A:164:ILE:HD12	0.55	2.02	23	1
1:A:126:TYR:O	1:A:127:ALA:HB3	0.55	2.02	8	3
1:A:125:VAL:HG12	1:A:130:LYS:HG2	0.55	1.78	13	2
1:A:18:TYR:O	1:A:18:TYR:CG	0.55	2.60	28	1
1:A:143:PHE:HE1	1:A:164:ILE:HG21	0.55	1.62	34	2
1:A:62:TYR:O	1:A:66:TYR:CD1	0.55	2.59	33	2
1:A:36:LEU:HD12	1:A:43:ASN:OD1	0.55	2.01	8	1
1:A:52:HIS:HB3	1:A:57:TYR:CE1	0.54	2.37	27	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:PHE:CD1	1:A:44:LEU:O	0.54	2.61	13	5
1:A:50:ALA:HB1	1:A:62:TYR:CZ	0.54	2.37	30	2
1:A:137:SER:C	1:A:138:TRP:CG	0.54	2.80	26	20
1:A:118:CYS:HB2	1:A:139:HIS:CE1	0.54	2.38	19	28
1:A:19:PHE:CG	1:A:19:PHE:O	0.54	2.60	35	2
1:A:62:TYR:CZ	1:A:66:TYR:OH	0.54	2.60	33	2
1:A:156:THR:HG22	1:A:156:THR:O	0.54	2.02	9	2
1:A:18:TYR:CG	1:A:18:TYR:O	0.54	2.60	36	1
1:A:35:PHE:CE2	1:A:49:VAL:HG21	0.54	2.37	29	1
1:A:121:CYS:SG	1:A:139:HIS:CE1	0.54	3.02	13	27
1:A:173:ASN:HB3	1:A:174:PHE:CD2	0.54	2.38	32	1
1:A:13:CYS:O	1:A:14:GLN:CB	0.53	2.56	22	36
1:A:47:THR:O	1:A:48:THR:CB	0.53	2.57	8	4
1:A:48:THR:HG22	1:A:48:THR:O	0.53	2.04	3	1
1:A:21:GLU:O	1:A:22:GLU:C	0.53	2.46	32	6
1:A:17:VAL:HG11	1:A:22:GLU:HB2	0.53	1.81	28	1
1:A:41:LYS:O	1:A:41:LYS:CD	0.53	2.57	34	1
1:A:28:SER:HB3	1:A:30:PHE:CZ	0.53	2.39	17	14
1:A:118:CYS:CB	1:A:139:HIS:ND1	0.53	2.72	19	2
1:A:40:CYS:O	1:A:41:LYS:CG	0.53	2.57	34	1
1:A:138:TRP:CE2	1:A:143:PHE:CE1	0.53	2.97	26	22
1:A:13:CYS:O	1:A:14:GLN:CG	0.53	2.57	10	1
1:A:143:PHE:CZ	1:A:157:LEU:HD21	0.53	2.39	27	3
1:A:35:PHE:HZ	1:A:49:VAL:HG11	0.52	1.63	16	8
1:A:29:SER:C	1:A:30:PHE:CD1	0.52	2.82	23	15
1:A:13:CYS:SG	1:A:31:HIS:CE1	0.52	3.02	17	2
1:A:157:LEU:HD12	1:A:158:ALA:H	0.52	1.64	34	6
1:A:119:PRO:CD	1:A:137:SER:O	0.52	2.58	25	12
1:A:37:CYS:N	1:A:44:LEU:CD1	0.52	2.73	37	1
1:A:14:GLN:O	1:A:14:GLN:CG	0.52	2.57	10	1
1:A:59:LYS:O	1:A:60:SER:C	0.52	2.48	18	36
1:A:52:HIS:HB3	1:A:57:TYR:CE2	0.52	2.40	26	10
1:A:158:ALA:HB1	1:A:170:TYR:CG	0.52	2.40	36	15
1:A:10:CYS:HB2	1:A:31:HIS:CE1	0.52	2.40	34	17
1:A:62:TYR:CE1	1:A:66:TYR:CE2	0.52	2.98	23	2
1:A:57:TYR:HB2	1:A:62:TYR:CE2	0.52	2.40	36	4
1:A:125:VAL:HG12	1:A:130:LYS:CG	0.52	2.35	20	6
1:A:35:PHE:CE1	1:A:56:ILE:CD1	0.52	2.92	16	1
1:A:156:THR:O	1:A:156:THR:HG22	0.52	2.05	12	3
1:A:10:CYS:CB	1:A:31:HIS:CE1	0.52	2.93	30	11
1:A:36:LEU:CD1	1:A:43:ASN:N	0.52	2.73	35	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:PRO:HG2	1:A:138:TRP:CE3	0.51	2.41	7	22
1:A:125:VAL:HG12	1:A:130:LYS:CB	0.51	2.35	26	3
1:A:131:VAL:HG23	1:A:140:LYS:NZ	0.51	2.20	16	1
1:A:18:TYR:O	1:A:19:PHE:CB	0.51	2.57	14	2
1:A:152:LEU:CD1	1:A:164:ILE:HD12	0.51	2.34	30	1
1:A:59:LYS:O	1:A:62:TYR:CB	0.51	2.59	10	13
1:A:116:ASP:CB	1:A:137:SER:OG	0.51	2.59	30	6
1:A:163:GLU:CB	1:A:165:TYR:CZ	0.51	2.94	35	4
1:A:15:LYS:NZ	1:A:16:ALA:H	0.51	2.04	8	1
1:A:142:CYS:O	1:A:143:PHE:C	0.51	2.49	21	33
1:A:36:LEU:C	1:A:56:ILE:CD1	0.51	2.79	18	2
1:A:25:CYS:SG	1:A:51:VAL:HG22	0.51	2.46	19	2
1:A:168:GLY:O	1:A:172:LYS:CG	0.50	2.60	14	6
1:A:25:CYS:SG	1:A:35:PHE:CZ	0.50	3.01	19	1
1:A:50:ALA:HB3	1:A:57:TYR:O	0.50	2.07	8	2
1:A:116:ASP:O	1:A:125:VAL:O	0.50	2.29	10	8
1:A:36:LEU:H	1:A:56:ILE:HD11	0.50	1.64	27	1
1:A:155:THR:HG22	1:A:155:THR:O	0.50	2.06	35	4
1:A:46:SER:O	1:A:47:THR:CG2	0.50	2.59	9	5
1:A:40:CYS:O	1:A:41:LYS:CB	0.50	2.58	18	29
1:A:35:PHE:CE2	1:A:49:VAL:HG11	0.50	2.41	29	1
1:A:44:LEU:O	1:A:45:ASP:CB	0.50	2.59	24	2
1:A:126:TYR:O	1:A:130:LYS:CD	0.50	2.59	13	2
1:A:169:CYS:O	1:A:173:ASN:CB	0.50	2.60	6	10
1:A:48:THR:O	1:A:59:LYS:CG	0.50	2.60	9	1
1:A:47:THR:O	1:A:47:THR:CG2	0.50	2.59	27	1
1:A:48:THR:O	1:A:59:LYS:CB	0.50	2.60	34	9
1:A:37:CYS:CA	1:A:44:LEU:HD12	0.50	2.37	25	2
1:A:55:GLU:CB	1:A:57:TYR:OH	0.50	2.59	36	3
1:A:116:ASP:CG	1:A:137:SER:CB	0.50	2.80	22	1
1:A:44:LEU:HD12	1:A:56:ILE:HG13	0.50	1.84	32	1
1:A:127:ALA:O	1:A:130:LYS:CD	0.50	2.60	34	1
1:A:47:THR:O	1:A:47:THR:HG23	0.50	2.06	16	2
1:A:62:TYR:CE2	1:A:66:TYR:CE2	0.50	2.99	24	2
1:A:52:HIS:CB	1:A:62:TYR:OH	0.50	2.59	36	1
1:A:158:ALA:CB	1:A:170:TYR:CG	0.49	2.95	26	9
1:A:19:PHE:O	1:A:20:ALA:CB	0.49	2.60	23	2
1:A:35:PHE:HE2	1:A:49:VAL:HG11	0.49	1.67	29	1
1:A:160:LYS:O	1:A:162:GLY:N	0.49	2.44	24	7
1:A:55:GLU:CB	1:A:57:TYR:CZ	0.49	2.95	36	2
1:A:48:THR:O	1:A:48:THR:CG2	0.49	2.61	14	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:THR:O	1:A:156:THR:CB	0.49	2.60	28	2
1:A:23:VAL:HG12	1:A:35:PHE:CD2	0.49	2.43	19	7
1:A:48:THR:CG2	1:A:48:THR:O	0.49	2.61	4	3
1:A:156:THR:HG23	1:A:156:THR:O	0.49	2.08	5	2
1:A:173:ASN:HB3	1:A:174:PHE:CE1	0.49	2.42	33	3
1:A:163:GLU:CB	1:A:165:TYR:OH	0.49	2.60	6	5
1:A:125:VAL:CG1	1:A:130:LYS:CG	0.49	2.90	20	1
1:A:52:HIS:HB2	1:A:57:TYR:CD2	0.49	2.43	37	2
1:A:55:GLU:HB3	1:A:57:TYR:CZ	0.49	2.42	36	17
1:A:152:LEU:O	1:A:153:GLU:CB	0.49	2.59	21	3
1:A:157:LEU:CD1	1:A:158:ALA:O	0.49	2.61	19	10
1:A:166:CYS:O	1:A:169:CYS:N	0.49	2.44	29	36
1:A:36:LEU:N	1:A:56:ILE:CD1	0.49	2.75	33	6
1:A:26:GLU:O	1:A:51:VAL:HG11	0.49	2.07	37	1
1:A:37:CYS:N	1:A:44:LEU:HD12	0.48	2.23	22	3
1:A:35:PHE:HE1	1:A:56:ILE:HD11	0.48	1.65	16	1
1:A:131:VAL:CG2	1:A:153:GLU:O	0.48	2.60	12	2
1:A:156:THR:HG22	1:A:167:LYS:HB2	0.48	1.85	19	1
1:A:36:LEU:HD21	1:A:41:LYS:HA	0.48	1.85	33	8
1:A:126:TYR:O	1:A:126:TYR:CG	0.48	2.66	16	2
1:A:125:VAL:HG12	1:A:130:LYS:HB2	0.48	1.85	26	2
1:A:140:LYS:O	1:A:140:LYS:CG	0.48	2.61	14	2
1:A:18:TYR:O	1:A:18:TYR:CD2	0.48	2.67	13	4
1:A:157:LEU:CD1	1:A:158:ALA:N	0.48	2.71	5	4
1:A:18:TYR:CD2	1:A:18:TYR:O	0.48	2.67	3	3
1:A:27:GLY:O	1:A:28:SER:CB	0.48	2.61	31	3
1:A:36:LEU:HD12	1:A:43:ASN:HA	0.48	1.85	16	1
1:A:30:PHE:CE2	1:A:56:ILE:CG2	0.48	2.96	27	1
1:A:39:VAL:CG2	1:A:57:TYR:CE1	0.48	2.97	30	1
1:A:163:GLU:HB3	1:A:165:TYR:CE2	0.48	2.44	7	8
1:A:36:LEU:N	1:A:56:ILE:HD12	0.48	2.24	18	2
1:A:28:SER:HB3	1:A:30:PHE:CE2	0.47	2.44	26	1
1:A:44:LEU:HD11	1:A:58:CYS:N	0.47	2.24	21	5
1:A:144:ARG:C	1:A:152:LEU:HD11	0.47	2.29	32	3
1:A:35:PHE:CD2	1:A:56:ILE:HD12	0.47	2.44	29	1
1:A:155:THR:O	1:A:155:THR:HG22	0.47	2.09	24	2
1:A:138:TRP:CZ2	1:A:164:ILE:HG21	0.47	2.44	13	4
1:A:48:THR:HG22	1:A:59:LYS:CG	0.47	2.39	31	1
1:A:18:TYR:CD1	1:A:18:TYR:O	0.47	2.66	36	1
1:A:163:GLU:HB3	1:A:165:TYR:CZ	0.47	2.44	6	35
1:A:154:SER:O	1:A:157:LEU:HD23	0.47	2.10	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:LYS:CD	1:A:22:GLU:OE2	0.47	2.62	28	1
1:A:127:ALA:O	1:A:128:ALA:CB	0.47	2.62	17	8
1:A:145:CYS:N	1:A:152:LEU:HD11	0.47	2.25	6	1
1:A:145:CYS:CB	1:A:152:LEU:HD21	0.47	2.40	33	2
1:A:52:HIS:HB2	1:A:57:TYR:CE1	0.47	2.44	27	1
1:A:138:TRP:CH2	1:A:164:ILE:HG12	0.47	2.44	17	9
1:A:174:PHE:CD1	1:A:175:GLY:N	0.47	2.83	32	1
1:A:168:GLY:O	1:A:172:LYS:CD	0.47	2.63	16	2
1:A:126:TYR:C	1:A:130:LYS:CE	0.47	2.83	13	2
1:A:51:VAL:C	1:A:62:TYR:HH	0.47	2.13	6	1
1:A:51:VAL:HG12	1:A:52:HIS:H	0.47	1.70	1	11
1:A:142:CYS:O	1:A:144:ARG:N	0.46	2.49	10	15
1:A:139:HIS:O	1:A:141:SER:N	0.46	2.48	21	12
1:A:59:LYS:O	1:A:62:TYR:N	0.46	2.49	23	22
1:A:61:CYS:O	1:A:64:LYS:N	0.46	2.48	35	21
1:A:37:CYS:HA	1:A:44:LEU:HD12	0.46	1.86	25	2
1:A:28:SER:HB2	1:A:30:PHE:CZ	0.46	2.45	28	2
1:A:153:GLU:N	1:A:153:GLU:CD	0.46	2.69	28	1
1:A:163:GLU:HG2	1:A:165:TYR:CZ	0.46	2.46	30	1
1:A:124:ALA:O	1:A:139:HIS:NE2	0.46	2.48	7	3
1:A:58:CYS:O	1:A:61:CYS:N	0.46	2.49	22	2
1:A:37:CYS:N	1:A:44:LEU:HD11	0.46	2.26	37	1
1:A:62:TYR:CZ	1:A:66:TYR:CZ	0.46	3.03	26	5
1:A:154:SER:O	1:A:156:THR:N	0.46	2.48	6	1
1:A:34:CYS:O	1:A:36:LEU:N	0.46	2.49	30	4
1:A:52:HIS:O	1:A:52:HIS:CD2	0.46	2.69	7	1
1:A:29:SER:O	1:A:30:PHE:CD1	0.46	2.68	30	1
1:A:157:LEU:C	1:A:157:LEU:CD1	0.46	2.84	17	3
1:A:161:ASP:O	1:A:163:GLU:N	0.46	2.49	30	1
1:A:172:LYS:C	1:A:174:PHE:N	0.46	2.69	16	9
1:A:46:SER:C	1:A:47:THR:HG23	0.46	2.31	9	6
1:A:125:VAL:O	1:A:126:TYR:CD1	0.46	2.69	21	1
1:A:173:ASN:HB3	1:A:174:PHE:CE2	0.45	2.46	32	1
1:A:47:THR:OG1	1:A:48:THR:N	0.45	2.48	12	2
1:A:156:THR:HG23	1:A:167:LYS:CG	0.45	2.40	12	2
1:A:50:ALA:CB	1:A:62:TYR:CD2	0.45	2.99	30	1
1:A:58:CYS:O	1:A:59:LYS:C	0.45	2.55	18	33
1:A:134:ALA:CB	1:A:159:ASP:CB	0.45	2.94	36	8
1:A:52:HIS:O	1:A:54:ASP:N	0.45	2.49	16	2
1:A:119:PRO:HG2	1:A:138:TRP:CZ3	0.45	2.46	37	1
1:A:28:SER:HB3	1:A:30:PHE:CE1	0.45	2.47	14	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:TRP:NE1	1:A:143:PHE:CE1	0.45	2.85	24	8
1:A:171:ALA:O	1:A:175:GLY:N	0.45	2.50	17	3
1:A:147:LYS:HB2	1:A:165:TYR:CD1	0.45	2.47	14	6
1:A:174:PHE:N	1:A:174:PHE:CD1	0.45	2.84	24	3
1:A:26:GLU:HB2	1:A:51:VAL:HG21	0.45	1.88	17	1
1:A:44:LEU:HD12	1:A:56:ILE:CG1	0.45	2.41	32	1
1:A:28:SER:HB2	1:A:30:PHE:CE2	0.45	2.47	28	1
1:A:22:GLU:CG	1:A:22:GLU:O	0.45	2.65	32	1
1:A:47:THR:HG23	1:A:48:THR:H	0.45	1.71	29	1
1:A:28:SER:CB	1:A:30:PHE:CE1	0.45	3.00	14	2
1:A:130:LYS:O	1:A:130:LYS:CG	0.45	2.65	16	2
1:A:62:TYR:CD1	1:A:66:TYR:CZ	0.45	3.05	5	2
1:A:144:ARG:CZ	1:A:149:GLY:O	0.44	2.65	17	1
1:A:157:LEU:CD1	1:A:157:LEU:C	0.44	2.80	20	3
1:A:173:ASN:HB3	1:A:174:PHE:CD1	0.44	2.47	16	1
1:A:62:TYR:CD2	1:A:66:TYR:CE2	0.44	3.05	34	1
1:A:25:CYS:O	1:A:26:GLU:C	0.44	2.56	21	8
1:A:139:HIS:C	1:A:141:SER:N	0.44	2.70	30	4
1:A:136:LYS:HE3	1:A:138:TRP:CH2	0.44	2.47	7	1
1:A:62:TYR:CE1	1:A:66:TYR:CE1	0.44	3.06	18	1
1:A:41:LYS:O	1:A:41:LYS:CG	0.44	2.65	34	1
1:A:25:CYS:CB	1:A:28:SER:OG	0.44	2.66	28	1
1:A:17:VAL:HG11	1:A:22:GLU:HG2	0.44	1.89	29	1
1:A:52:HIS:C	1:A:52:HIS:CD2	0.44	2.91	34	1
1:A:153:GLU:O	1:A:154:SER:CB	0.44	2.65	17	1
1:A:25:CYS:SG	1:A:49:VAL:CG1	0.44	3.06	26	1
1:A:172:LYS:O	1:A:174:PHE:N	0.44	2.51	20	8
1:A:35:PHE:C	1:A:56:ILE:HD13	0.44	2.33	8	1
1:A:8:LYS:CD	1:A:22:GLU:CD	0.44	2.86	37	1
1:A:35:PHE:HA	1:A:56:ILE:CD1	0.44	2.43	22	2
1:A:155:THR:O	1:A:156:THR:CG2	0.44	2.65	27	2
1:A:160:LYS:HE3	1:A:174:PHE:CZ	0.44	2.48	7	1
1:A:8:LYS:CB	1:A:22:GLU:OE2	0.43	2.66	33	1
1:A:161:ASP:C	1:A:163:GLU:N	0.43	2.71	30	1
1:A:39:VAL:HG11	1:A:61:CYS:HB3	0.43	1.90	21	1
1:A:125:VAL:CG1	1:A:130:LYS:CB	0.43	2.96	26	1
1:A:48:THR:OG1	1:A:59:LYS:CB	0.43	2.67	16	2
1:A:52:HIS:HB2	1:A:57:TYR:CD1	0.43	2.49	27	1
1:A:17:VAL:HG12	1:A:22:GLU:HB3	0.43	1.90	24	1
1:A:160:LYS:O	1:A:161:ASP:C	0.43	2.56	7	16
1:A:171:ALA:O	1:A:174:PHE:C	0.43	2.57	8	33

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:CYS:HB3	1:A:30:PHE:CE2	0.43	2.47	12	2
1:A:47:THR:O	1:A:48:THR:CG2	0.43	2.65	25	2
1:A:52:HIS:CD2	1:A:52:HIS:O	0.43	2.72	22	1
1:A:126:TYR:N	1:A:126:TYR:CD1	0.43	2.86	19	1
1:A:172:LYS:O	1:A:173:ASN:C	0.43	2.57	5	31
1:A:126:TYR:O	1:A:130:LYS:CG	0.43	2.67	13	2
1:A:155:THR:HG22	1:A:156:THR:N	0.43	2.28	18	1
1:A:173:ASN:OD1	1:A:174:PHE:CE1	0.43	2.72	27	1
1:A:154:SER:CA	1:A:157:LEU:HD23	0.43	2.42	1	2
1:A:35:PHE:HE1	1:A:49:VAL:HG11	0.43	1.73	33	1
1:A:48:THR:HG23	1:A:59:LYS:CE	0.43	2.43	23	1
1:A:19:PHE:O	1:A:20:ALA:C	0.43	2.57	14	2
1:A:134:ALA:CB	1:A:159:ASP:HB2	0.43	2.44	18	7
1:A:18:TYR:CE2	1:A:20:ALA:HB3	0.43	2.49	13	2
1:A:50:ALA:O	1:A:57:TYR:O	0.43	2.37	16	1
1:A:130:LYS:O	1:A:130:LYS:CD	0.43	2.67	16	1
1:A:19:PHE:CG	1:A:20:ALA:N	0.43	2.86	12	2
1:A:51:VAL:HG13	1:A:55:GLU:O	0.43	2.13	10	1
1:A:23:VAL:HG21	1:A:32:LYS:HA	0.43	1.90	33	1
1:A:134:ALA:CB	1:A:159:ASP:HB3	0.43	2.44	10	7
1:A:23:VAL:CG1	1:A:35:PHE:CD1	0.43	3.00	29	1
1:A:21:GLU:O	1:A:21:GLU:CG	0.43	2.67	10	1
1:A:118:CYS:HB2	1:A:125:VAL:CG2	0.42	2.44	27	9
1:A:174:PHE:CD1	1:A:174:PHE:N	0.42	2.86	26	4
1:A:127:ALA:N	1:A:130:LYS:NZ	0.42	2.66	13	2
1:A:116:ASP:OD2	1:A:137:SER:CB	0.42	2.67	22	1
1:A:52:HIS:CD2	1:A:66:TYR:OH	0.42	2.72	29	1
1:A:155:THR:CG2	1:A:156:THR:HG23	0.42	2.34	16	1
1:A:46:SER:O	1:A:47:THR:HG23	0.42	2.13	9	1
1:A:51:VAL:HG12	1:A:52:HIS:N	0.42	2.29	1	11
1:A:143:PHE:CZ	1:A:157:LEU:HD22	0.42	2.49	23	2
1:A:47:THR:O	1:A:48:THR:C	0.42	2.57	14	2
1:A:18:TYR:CE2	1:A:20:ALA:HB2	0.42	2.49	36	1
1:A:8:LYS:NZ	1:A:9:LYS:H	0.42	2.11	29	1
1:A:30:PHE:CD1	1:A:30:PHE:N	0.42	2.87	29	1
1:A:125:VAL:CG1	1:A:130:LYS:HA	0.42	2.44	1	5
1:A:154:SER:O	1:A:155:THR:C	0.42	2.57	17	1
1:A:13:CYS:C	1:A:14:GLN:CG	0.42	2.86	26	1
1:A:18:TYR:CE1	1:A:19:PHE:CE2	0.42	3.07	34	1
1:A:126:TYR:CG	1:A:127:ALA:N	0.42	2.88	10	1
1:A:155:THR:HG23	1:A:155:THR:O	0.42	2.14	36	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:GLU:C	1:A:22:GLU:CD	0.42	2.78	1	2
1:A:52:HIS:CD2	1:A:66:TYR:HH	0.42	2.32	29	1
1:A:36:LEU:CA	1:A:56:ILE:HD11	0.42	2.44	35	1
1:A:143:PHE:CZ	1:A:157:LEU:CD2	0.42	3.02	21	2
1:A:52:HIS:O	1:A:57:TYR:CE2	0.42	2.73	23	1
1:A:124:ALA:HB1	1:A:126:TYR:CZ	0.42	2.50	21	1
1:A:52:HIS:ND1	1:A:57:TYR:CZ	0.41	2.88	34	1
1:A:125:VAL:CG1	1:A:130:LYS:HG2	0.41	2.45	20	2
1:A:155:THR:HG23	1:A:156:THR:H	0.41	1.73	16	1
1:A:60:SER:O	1:A:61:CYS:C	0.41	2.58	12	9
1:A:36:LEU:N	1:A:56:ILE:HD13	0.41	2.30	33	1
1:A:38:MET:HB2	1:A:57:TYR:CE1	0.41	2.50	18	1
1:A:98:HIS:CG	1:A:99:ARG:N	0.41	2.88	18	1
1:A:35:PHE:CD1	1:A:44:LEU:HB3	0.41	2.50	25	1
1:A:152:LEU:O	1:A:153:GLU:CD	0.41	2.58	17	1
1:A:142:CYS:O	1:A:144:ARG:CD	0.41	2.68	7	2
1:A:39:VAL:CG2	1:A:57:TYR:CD2	0.41	3.04	35	1
1:A:125:VAL:CG1	1:A:130:LYS:HG3	0.41	2.45	20	1
1:A:157:LEU:HD12	1:A:158:ALA:C	0.41	2.35	5	2
1:A:30:PHE:CZ	1:A:56:ILE:CG2	0.41	3.02	27	1
1:A:156:THR:CG2	1:A:167:LYS:HG2	0.41	2.46	35	1
1:A:49:VAL:HG22	1:A:50:ALA:H	0.41	1.74	16	1
1:A:48:THR:HG22	1:A:59:LYS:HB3	0.41	1.91	23	2
1:A:126:TYR:O	1:A:127:ALA:C	0.41	2.59	13	2
1:A:45:ASP:O	1:A:46:SER:C	0.41	2.59	14	2
1:A:158:ALA:HB2	1:A:170:TYR:HB2	0.41	1.93	18	1
1:A:152:LEU:HD22	1:A:165:TYR:O	0.41	2.16	1	2
1:A:35:PHE:CE1	1:A:44:LEU:HB2	0.41	2.51	34	1
1:A:127:ALA:O	1:A:130:LYS:CG	0.41	2.68	34	1
1:A:144:ARG:NE	1:A:149:GLY:O	0.41	2.54	17	1
1:A:143:PHE:O	1:A:152:LEU:CB	0.41	2.68	35	1
1:A:55:GLU:HB3	1:A:57:TYR:CE1	0.41	2.51	23	2
1:A:173:ASN:ND2	1:A:174:PHE:CE1	0.41	2.89	7	1
1:A:53:GLY:O	1:A:54:ASP:C	0.41	2.58	10	1
1:A:51:VAL:C	1:A:62:TYR:OH	0.41	2.58	6	1
1:A:140:LYS:CG	1:A:140:LYS:O	0.41	2.69	20	1
1:A:160:LYS:HE2	1:A:174:PHE:CE2	0.41	2.51	17	1
1:A:149:GLY:O	1:A:150:LYS:O	0.41	2.39	17	1
1:A:22:GLU:CD	1:A:22:GLU:O	0.41	2.59	32	1
1:A:134:ALA:HA	1:A:159:ASP:CB	0.41	2.46	36	5
1:A:127:ALA:O	1:A:128:ALA:C	0.41	2.59	16	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:O	1:A:38:MET:SD	0.41	2.79	29	1
1:A:154:SER:O	1:A:155:THR:O	0.41	2.39	29	1
1:A:8:LYS:O	1:A:17:VAL:HG23	0.41	2.16	23	1
1:A:35:PHE:C	1:A:56:ILE:HD11	0.41	2.36	23	1
1:A:128:ALA:C	1:A:129:GLU:CD	0.41	2.80	12	2
1:A:138:TRP:CE2	1:A:143:PHE:CZ	0.41	3.08	6	1
1:A:134:ALA:O	1:A:135:GLY:C	0.41	2.59	27	1
1:A:66:TYR:O	1:A:67:GLY:C	0.41	2.60	31	7
1:A:169:CYS:O	1:A:173:ASN:OD1	0.41	2.38	32	3
1:A:52:HIS:HB3	1:A:57:TYR:CD1	0.41	2.51	33	2
1:A:44:LEU:O	1:A:45:ASP:CG	0.41	2.60	26	1
1:A:25:CYS:SG	1:A:51:VAL:CG2	0.41	3.09	31	1
1:A:48:THR:OG1	1:A:59:LYS:CD	0.41	2.69	35	1
1:A:52:HIS:CE1	1:A:66:TYR:OH	0.41	2.74	12	2
1:A:156:THR:O	1:A:157:LEU:O	0.40	2.39	29	1
1:A:17:VAL:CG1	1:A:22:GLU:HG2	0.40	2.46	29	1
1:A:140:LYS:CG	1:A:153:GLU:HB3	0.40	2.46	29	1
1:A:16:ALA:O	1:A:31:HIS:NE2	0.40	2.49	16	1
1:A:143:PHE:CZ	1:A:164:ILE:HG21	0.40	2.51	18	1
1:A:18:TYR:O	1:A:19:PHE:C	0.40	2.60	5	4
1:A:158:ALA:CB	1:A:170:TYR:HB2	0.40	2.46	33	1
1:A:127:ALA:O	1:A:128:ALA:O	0.40	2.40	8	3
1:A:155:THR:C	1:A:157:LEU:N	0.40	2.75	6	1
1:A:102:ASN:O	1:A:102:ASN:CG	0.40	2.60	6	1
1:A:144:ARG:O	1:A:145:CYS:C	0.40	2.60	24	1
1:A:132:ILE:CD1	1:A:137:SER:HB2	0.40	2.47	26	1
1:A:153:GLU:O	1:A:154:SER:C	0.40	2.59	31	1
1:A:155:THR:C	1:A:156:THR:CG2	0.40	2.90	7	1
1:A:18:TYR:CZ	1:A:20:ALA:HB3	0.40	2.50	36	1
1:A:21:GLU:O	1:A:22:GLU:O	0.40	2.40	32	1
1:A:47:THR:HG23	1:A:48:THR:N	0.40	2.32	29	1
1:A:173:ASN:C	1:A:174:PHE:CD1	0.40	2.95	13	2
1:A:31:HIS:O	1:A:34:CYS:N	0.40	2.54	23	1
1:A:118:CYS:HB3	1:A:139:HIS:CE1	0.40	2.51	19	1
1:A:36:LEU:O	1:A:37:CYS:C	0.40	2.60	37	1
1:A:126:TYR:C	1:A:130:LYS:NZ	0.40	2.75	13	2
1:A:131:VAL:CG2	1:A:154:SER:OG	0.40	2.70	14	2
1:A:47:THR:HG23	1:A:48:THR:OG1	0.40	2.17	18	1
1:A:25:CYS:O	1:A:28:SER:O	0.40	2.40	25	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	137/192 (71%)	91±5 (66±3%)	36±4 (26±3%)	10±2 (8±2%)	3	16
All	All	5069/7104 (71%)	3350 (66%)	1337 (26%)	382 (8%)	3	16

All 45 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	143	PHE	36
1	A	67	GLY	30
1	A	20	ALA	22
1	A	19	PHE	21
1	A	128	ALA	19
1	A	154	SER	16
1	A	26	GLU	16
1	A	47	THR	16
1	A	153	GLU	15
1	A	46	SER	15
1	A	53	GLY	15
1	A	141	SER	14
1	A	14	GLN	11
1	A	35	PHE	11
1	A	45	ASP	10
1	A	22	GLU	10
1	A	156	THR	8
1	A	126	TYR	8
1	A	161	ASP	8
1	A	175	GLY	7
1	A	48	THR	7
1	A	155	THR	6
1	A	127	ALA	6
1	A	129	GLU	6
1	A	115	SER	5
1	A	28	SER	4
1	A	54	ASP	4

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Mol	Chain	Res	Type	Models (Total)
1	A	123	GLN	4
1	A	41	LYS	4
1	A	8	LYS	3
1	A	124	ALA	3
1	A	21	GLU	3
1	A	102	ASN	3
1	A	31	HIS	2
1	A	29	SER	2
1	A	60	SER	2
1	A	140	LYS	2
1	A	150	LYS	1
1	A	109	ALA	1
1	A	33	SER	1
1	A	174	PHE	1
1	A	18	TYR	1
1	A	157	LEU	1
1	A	105	ALA	1
1	A	162	GLY	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	111/146 (76%)	77±4 (69±4%)	34±4 (31±4%)	2	16
All	All	4107/5402 (76%)	2842 (69%)	1265 (31%)	2	16

All 78 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	138	TRP	37
1	A	152	LEU	37
1	A	157	LEU	35
1	A	56	ILE	34
1	A	160	LYS	33
1	A	64	LYS	30
1	A	107	ARG	30

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Mol	Chain	Res	Type	Models (Total)
1	A	36	LEU	29
1	A	59	LYS	29
1	A	38	MET	29
1	A	25	CYS	25
1	A	147	LYS	25
1	A	42	LYS	25
1	A	8	LYS	25
1	A	55	GLU	24
1	A	28	SER	23
1	A	116	ASP	23
1	A	129	GLU	23
1	A	99	ARG	22
1	A	120	ARG	21
1	A	96	GLN	21
1	A	150	LYS	20
1	A	9	LYS	20
1	A	30	PHE	20
1	A	41	LYS	20
1	A	62	TYR	20
1	A	167	LYS	20
1	A	108	MET	20
1	A	141	SER	20
1	A	136	LYS	19
1	A	130	LYS	19
1	A	26	GLU	18
1	A	45	ASP	17
1	A	98	HIS	17
1	A	14	GLN	17
1	A	33	SER	17
1	A	144	ARG	17
1	A	15	LYS	17
1	A	97	SER	17
1	A	143	PHE	16
1	A	123	GLN	16
1	A	60	SER	16
1	A	153	GLU	15
1	A	46	SER	15
1	A	140	LYS	15
1	A	154	SER	14
1	A	94	GLU	14
1	A	24	GLN	14
1	A	32	LYS	13

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Mol	Chain	Res	Type	Models (Total)
1	A	52	HIS	13
1	A	65	LYS	13
1	A	159	ASP	13
1	A	106	SER	12
1	A	137	SER	11
1	A	35	PHE	11
1	A	22	GLU	11
1	A	21	GLU	10
1	A	161	ASP	10
1	A	19	PHE	9
1	A	151	SER	9
1	A	104	ASN	8
1	A	18	TYR	8
1	A	172	LYS	8
1	A	43	ASN	7
1	A	54	ASP	7
1	A	115	SER	6
1	A	163	GLU	5
1	A	156	THR	5
1	A	142	CYS	5
1	A	102	ASN	4
1	A	47	THR	4
1	A	29	SER	3
1	A	170	TYR	2
1	A	44	LEU	2
1	A	164	ILE	2
1	A	174	PHE	2
1	A	48	THR	1
1	A	57	TYR	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 [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided