Full wwPDB NMR Structure Validation Report (i)

May 28, 2020 – 07:48 pm BST

PDB ID	:	1E5G
Title	:	Solution structure of central CP module pair of a pox virus complement inhibitor
Authors	:	Henderson, C.E.; Bromek, K.; Mullin, N.P.; Smith, B.O.; Uhrin, D.; Barlow, P.N.
Deposited on	:	2000-07-25

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

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

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

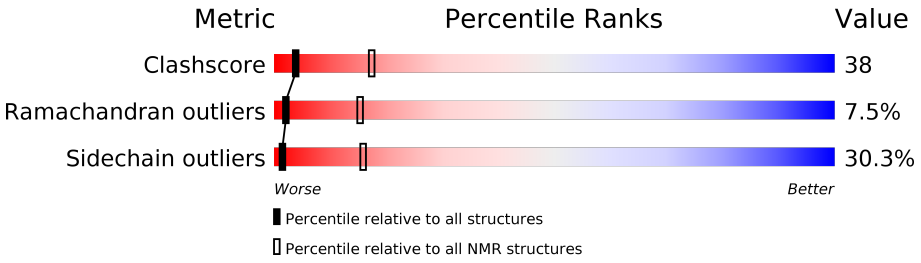
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	120	27% 55% 10% 8%

2 Ensemble composition and analysis

This entry contains 50 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 37 as representative.

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:51, A:57-A:68 (56)	0.26	13
2	A:69-A:83, A:88-A:126 (54)	0.23	9

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 10 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 30, 31, 32, 35, 39, 43, 46, 50
2	2, 7, 22, 23, 24, 27, 37, 40, 41, 47
3	9, 20, 25, 36, 42
4	10, 18, 28, 33, 34
5	11, 16, 17, 49
6	8, 13, 48
7	5, 6, 15
8	26, 45
9	12, 44
10	14, 19
Single-model clusters	21; 29; 38

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1698 atoms, of which 807 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called COMPLEMENT CONTROL PROTEIN C3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	120	1698	544	807	150	188	9	0

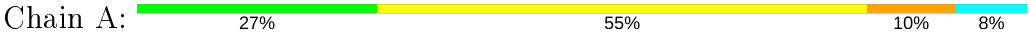
4 Residue-property plots

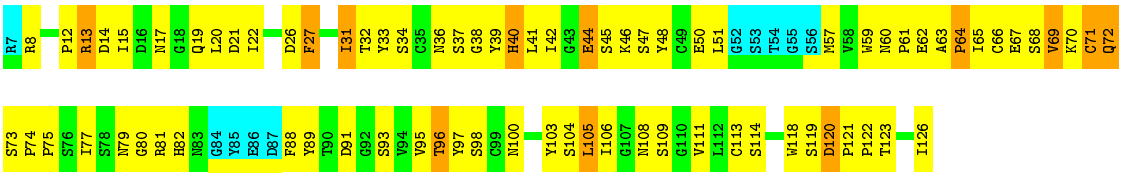
4.1 Average score per residue in the NMR ensemble

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: COMPLEMENT CONTROL PROTEIN C3

Chain A:





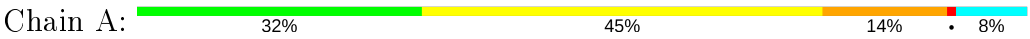
4.2 Scores per residue for each member of the ensemble

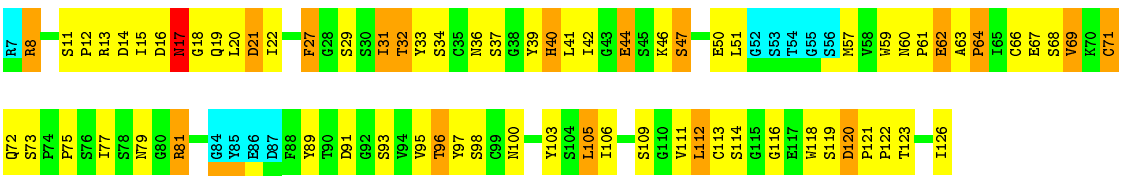
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

Chain A:

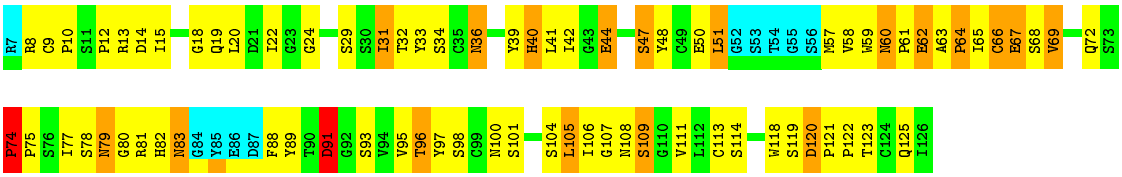




4.2.2 Score per residue for model 2

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

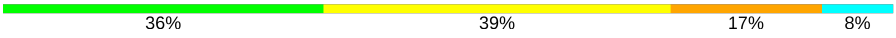
Chain A:

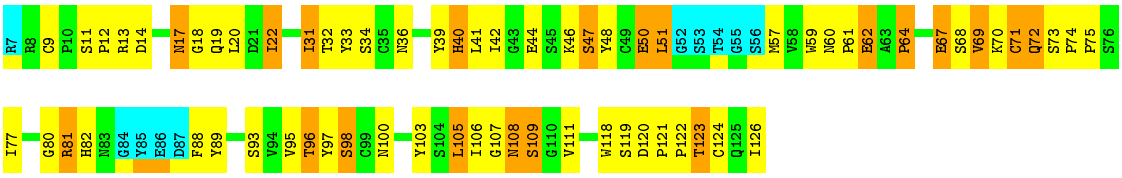


4.2.3 Score per residue for model 3

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

Chain A:

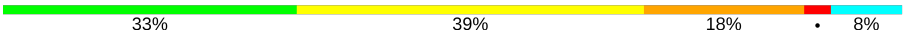


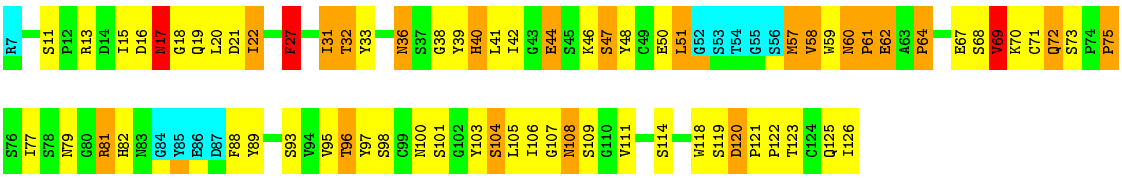


4.2.4 Score per residue for model 4

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

Chain A:

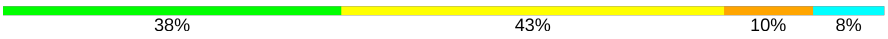


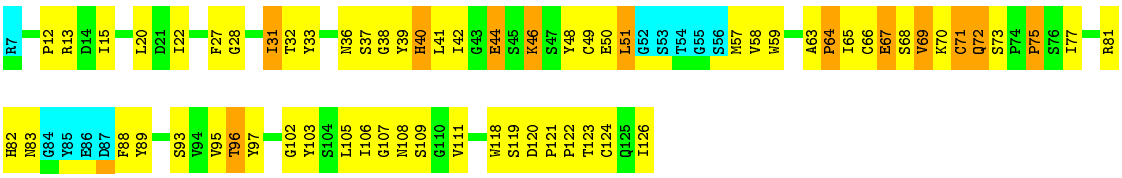


4.2.5 Score per residue for model 5

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

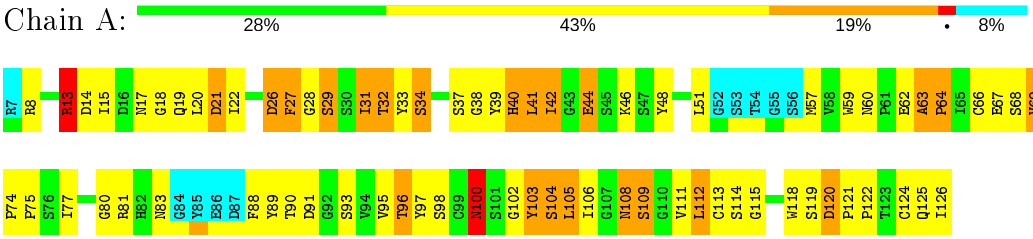
Chain A:





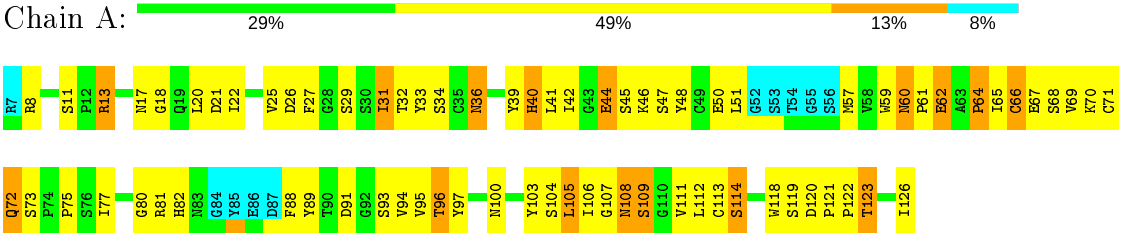
4.2.6 Score per residue for model 6

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3



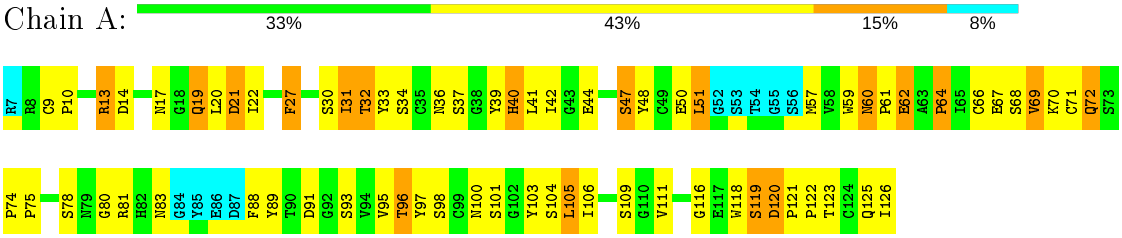
4.2.7 Score per residue for model 7

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



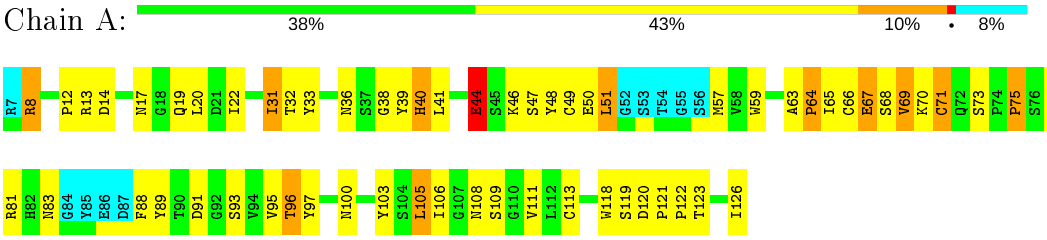
4.2.8 Score per residue for model 8

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



4.2.9 Score per residue for model 9

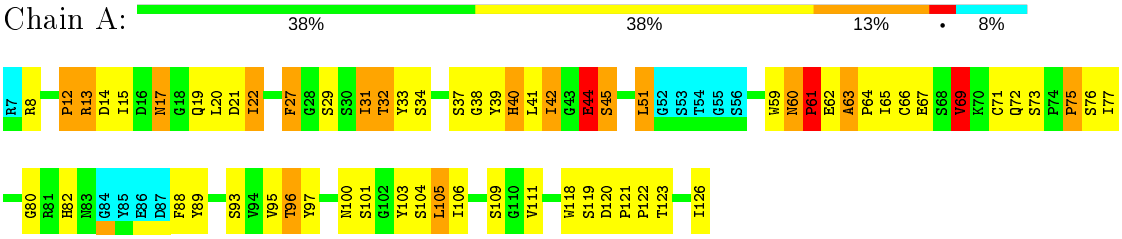
- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



4.2.10 Score per residue for model 10

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

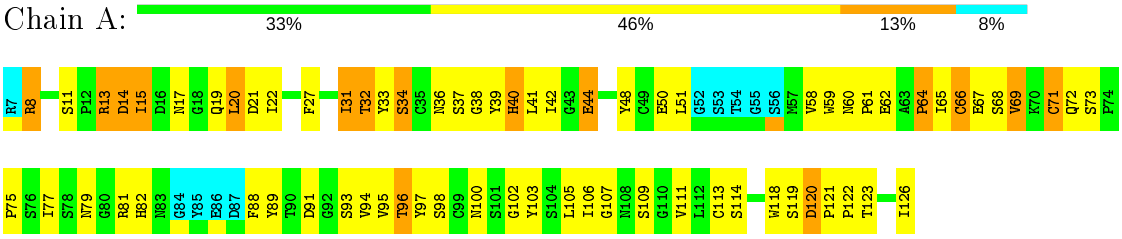
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

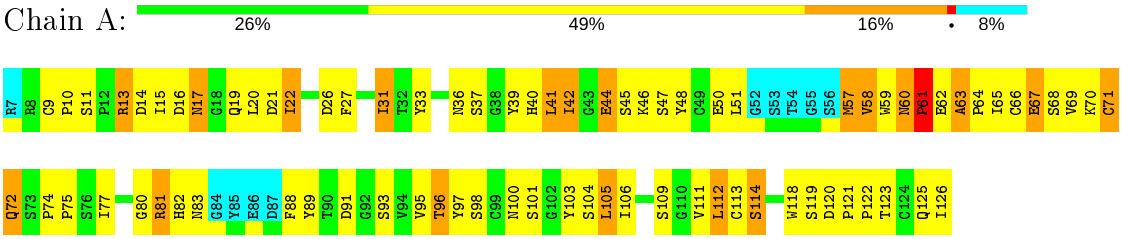
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

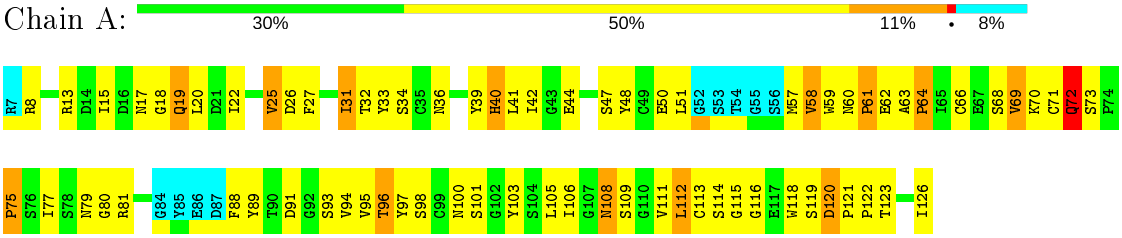
Chain A:



4.2.13 Score per residue for model 13 (medoid)

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

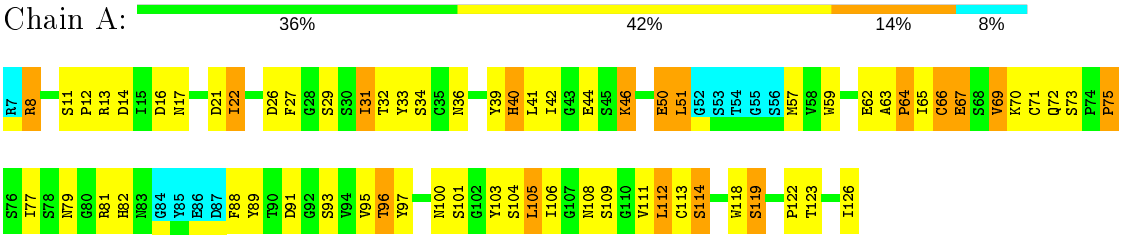
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

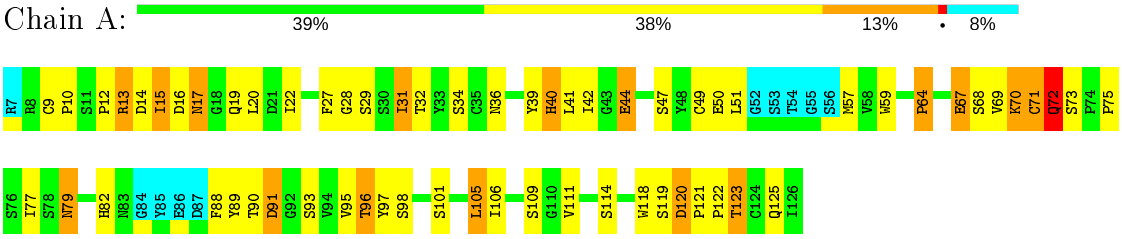
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

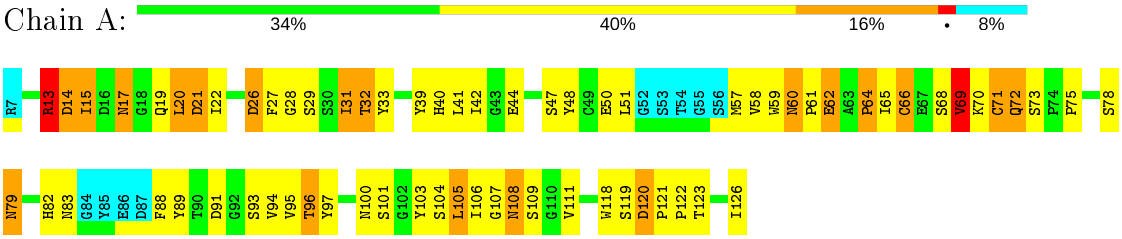
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

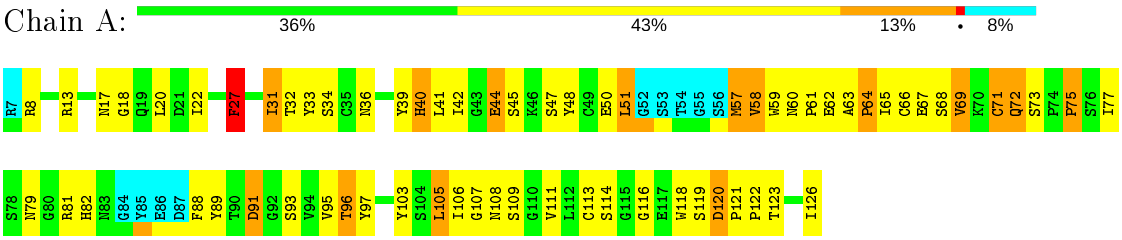
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

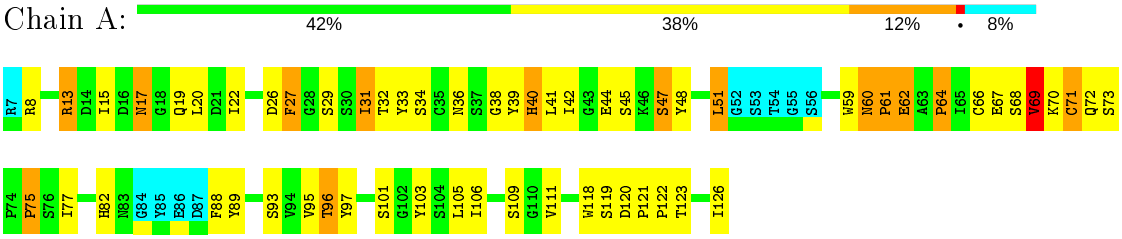
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

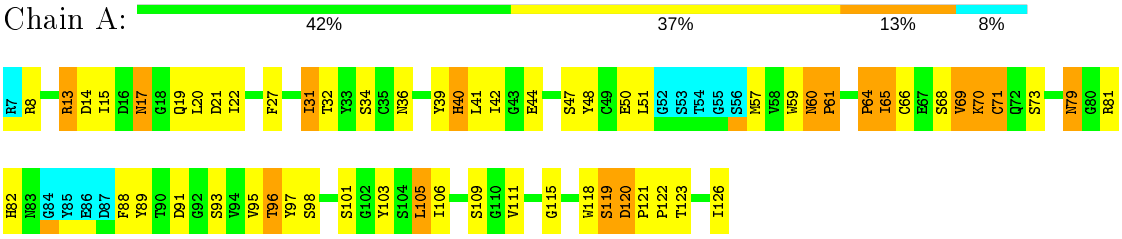
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

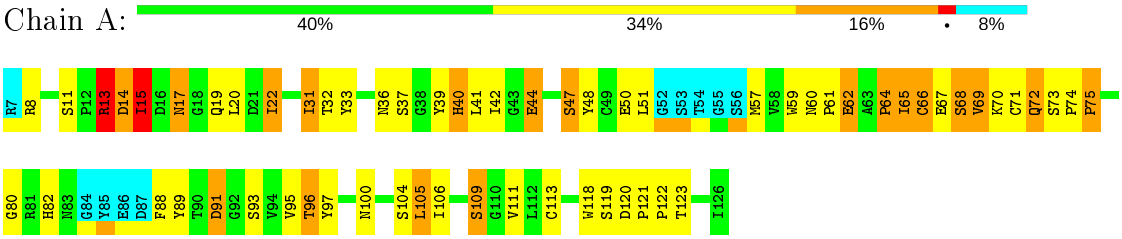
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

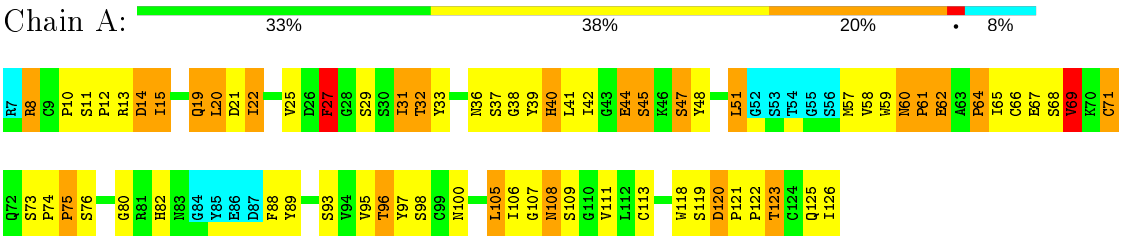
Chain A:



4.2.21 Score per residue for model 21

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

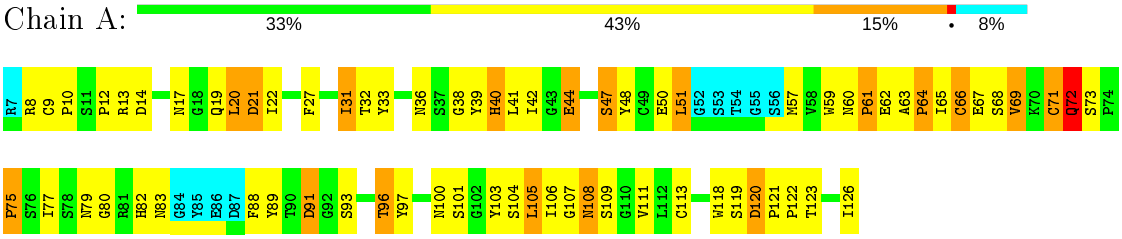
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

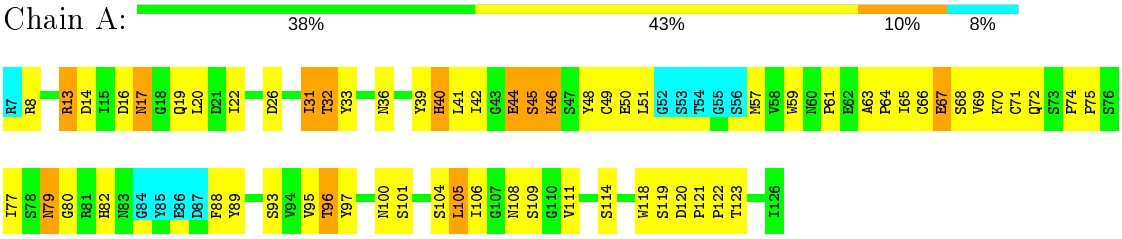
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

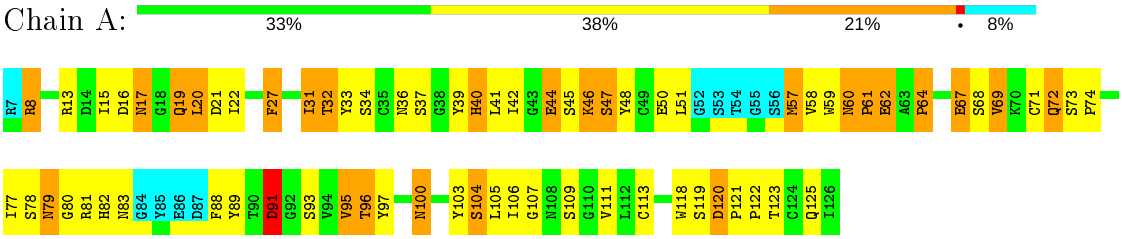
Chain A:



4.2.24 Score per residue for model 24

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

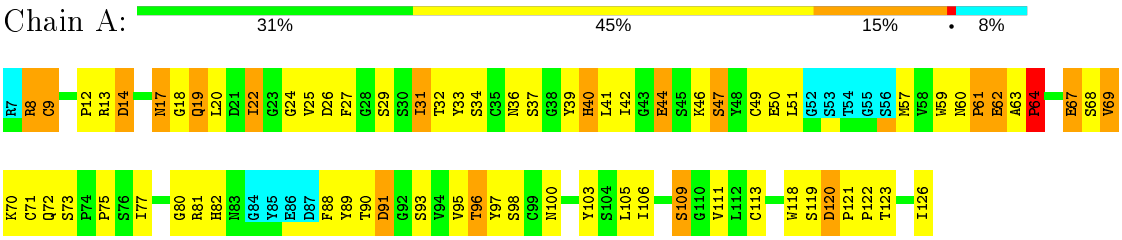
Chain A:



4.2.25 Score per residue for model 25

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

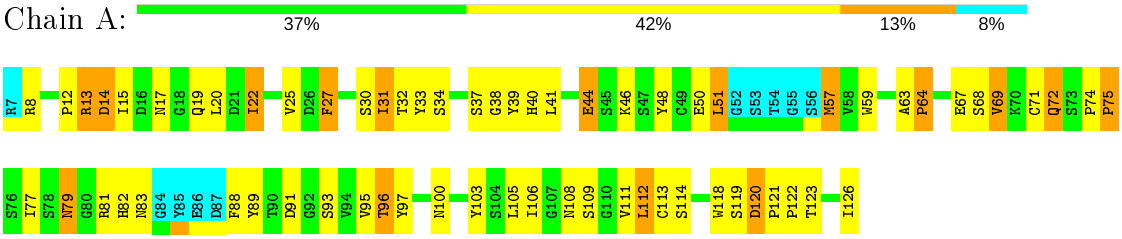
Chain A:



4.2.26 Score per residue for model 26

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

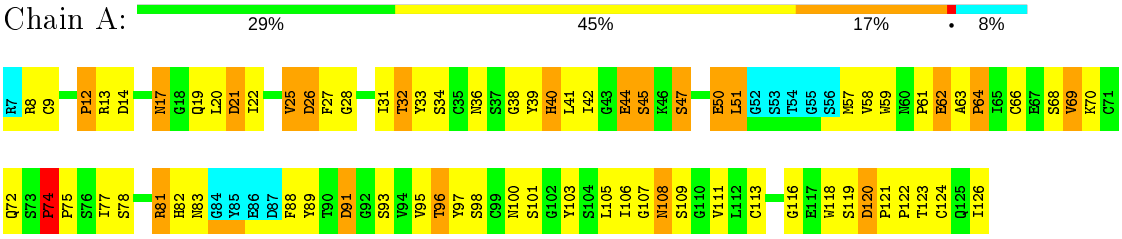
Chain A:



4.2.27 Score per residue for model 27

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

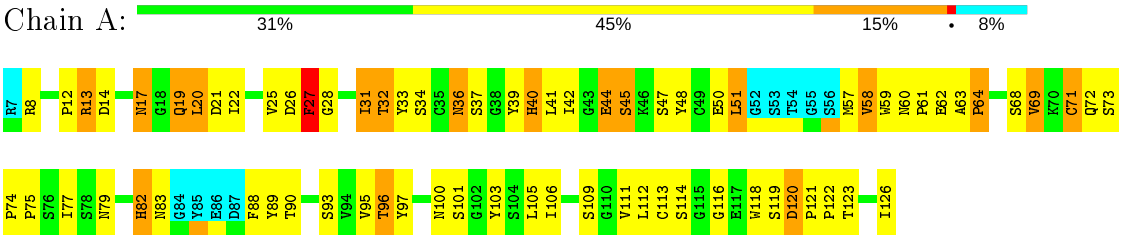
Chain A:



4.2.28 Score per residue for model 28

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

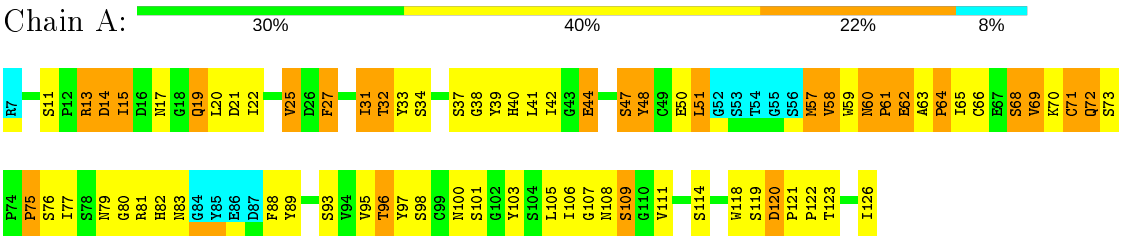
Chain A:



4.2.29 Score per residue for model 29

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

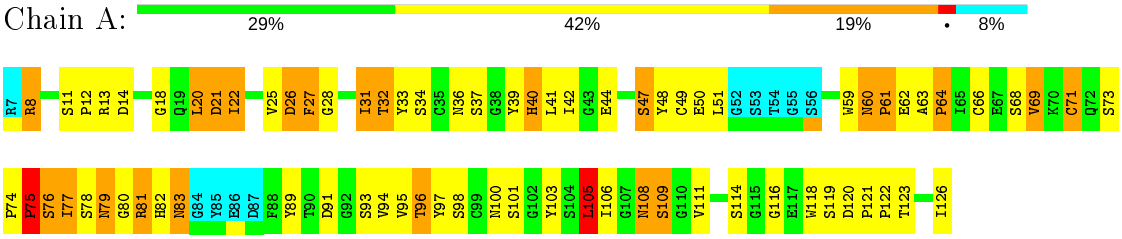
Chain A:



4.2.30 Score per residue for model 30

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

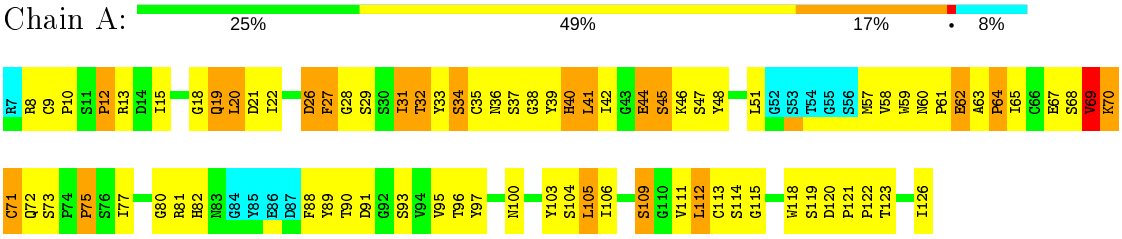
Chain A:



4.2.31 Score per residue for model 31

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

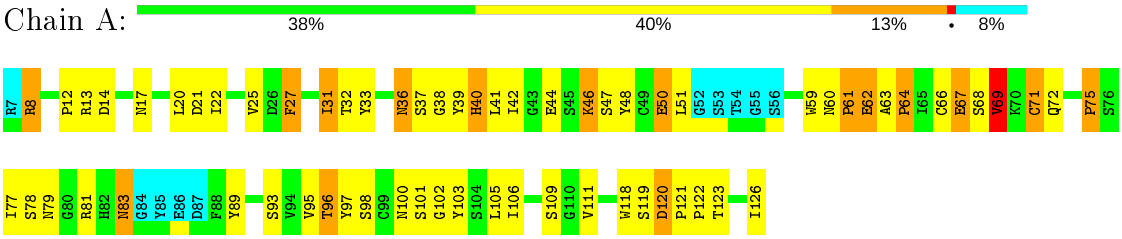
Chain A:



4.2.32 Score per residue for model 32

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

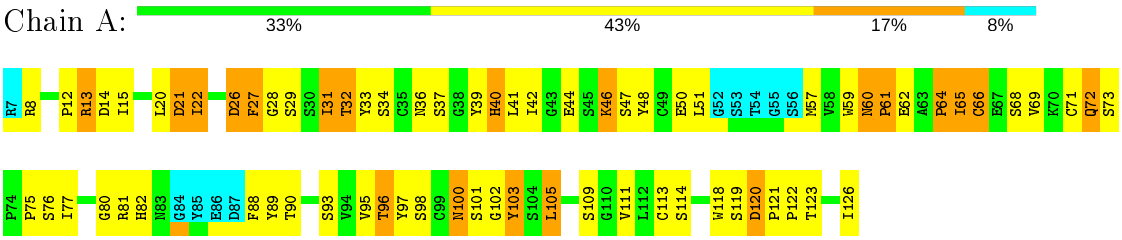
Chain A:



4.2.33 Score per residue for model 33

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

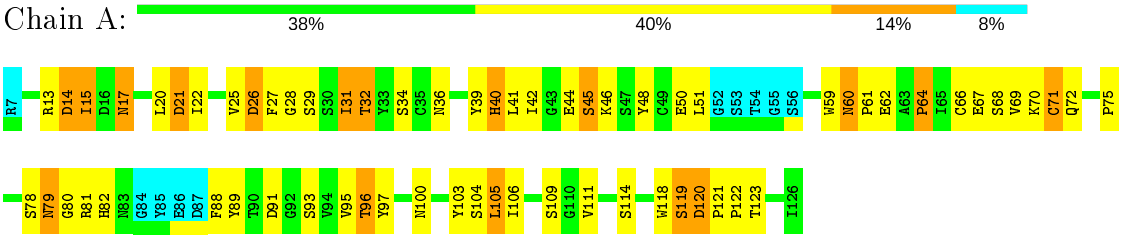
Chain A:



4.2.34 Score per residue for model 34

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

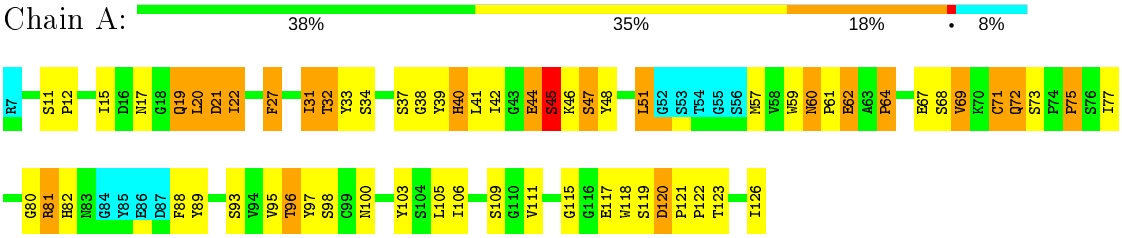
Chain A:



4.2.35 Score per residue for model 35

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

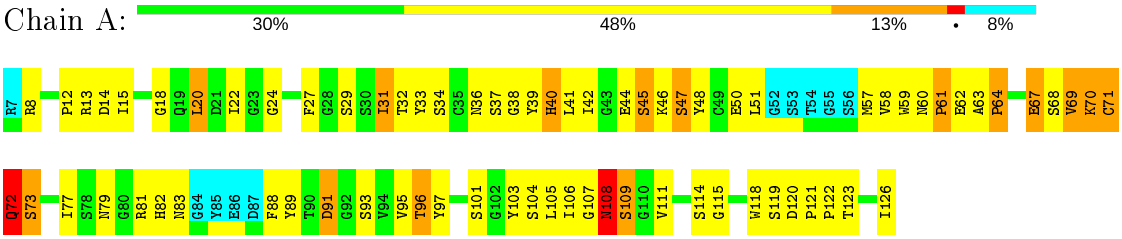
Chain A:



4.2.36 Score per residue for model 36

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

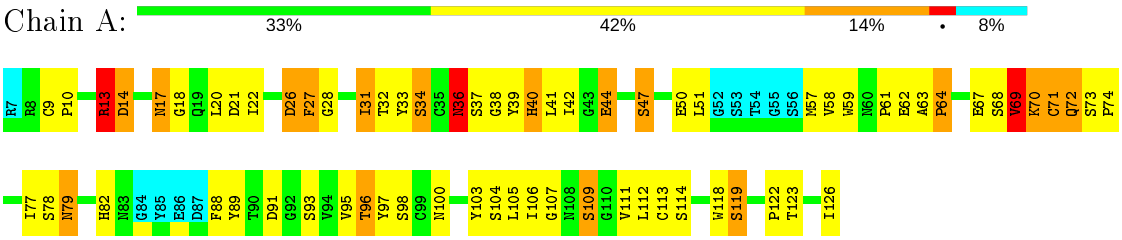
Chain A:



4.2.37 Score per residue for model 37

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

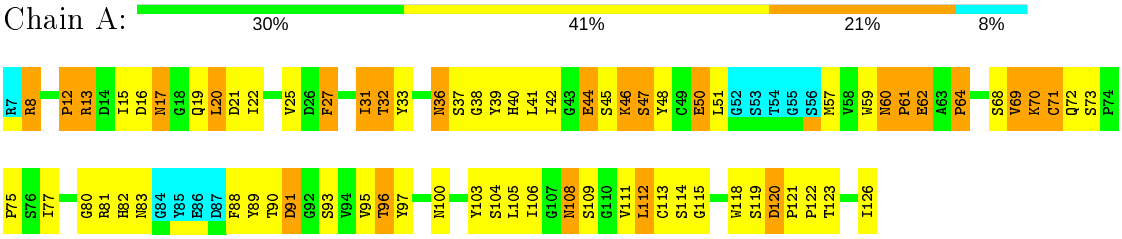
Chain A:



4.2.38 Score per residue for model 38

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

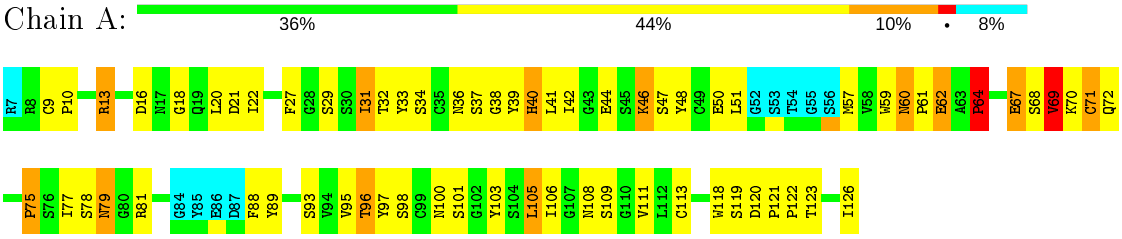
Chain A:



4.2.39 Score per residue for model 39

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

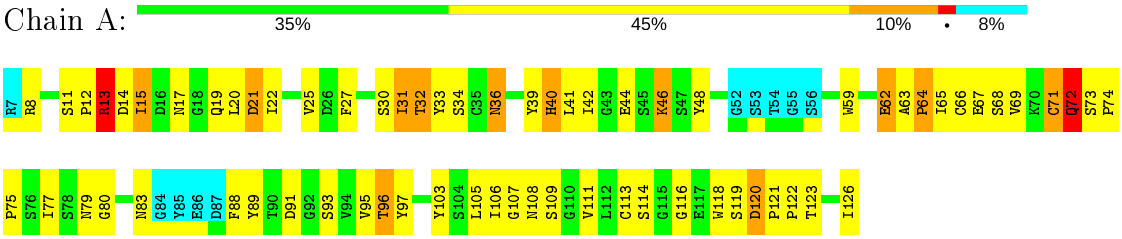
Chain A:



4.2.40 Score per residue for model 40

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

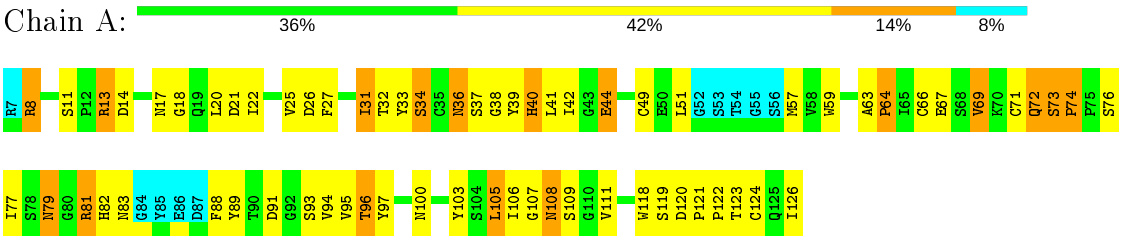
Chain A:



4.2.41 Score per residue for model 41

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

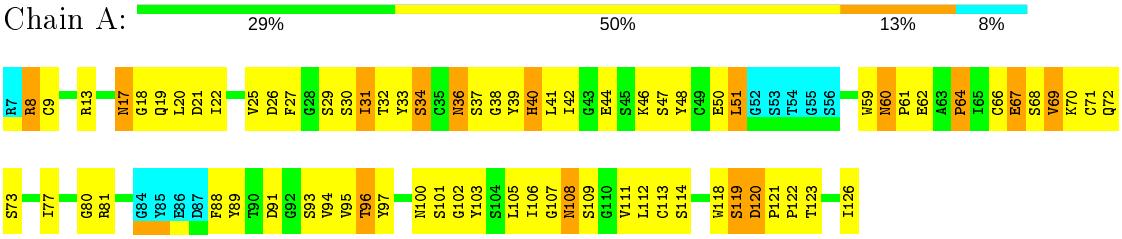
Chain A:



4.2.42 Score per residue for model 42

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

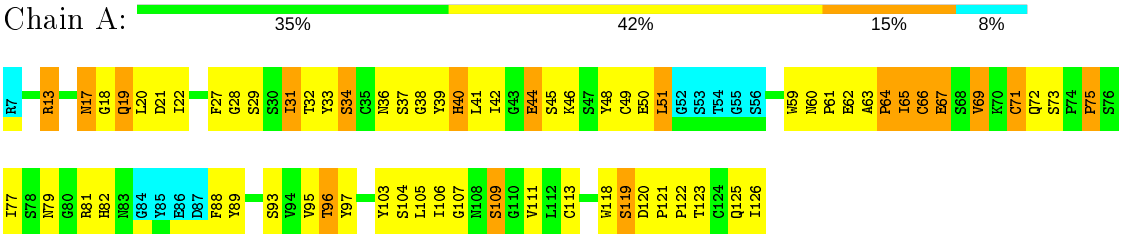
Chain A:



4.2.43 Score per residue for model 43

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

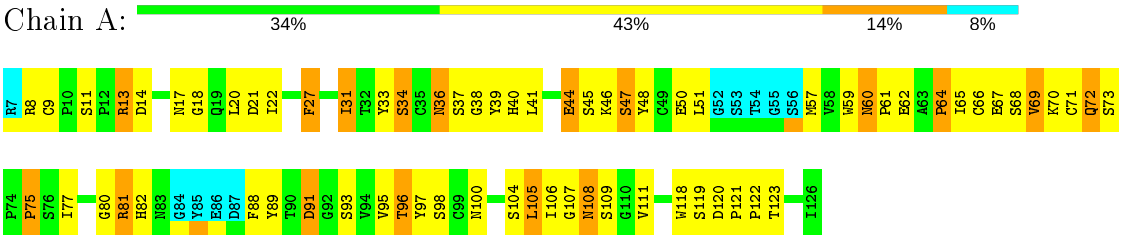
Chain A:



4.2.44 Score per residue for model 44

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

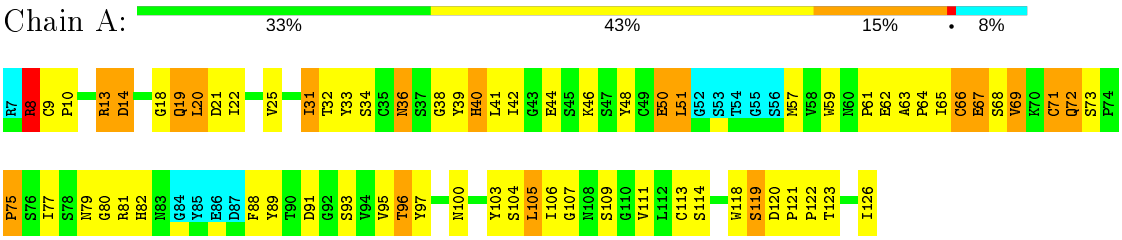
Chain A:



4.2.45 Score per residue for model 45

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

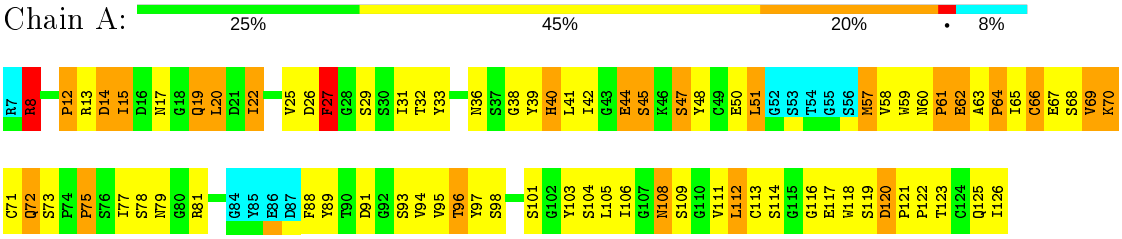
Chain A:



4.2.46 Score per residue for model 46

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

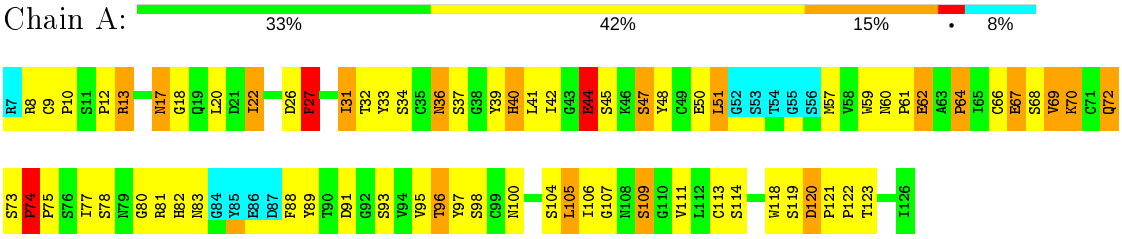
Chain A:



4.2.47 Score per residue for model 47

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

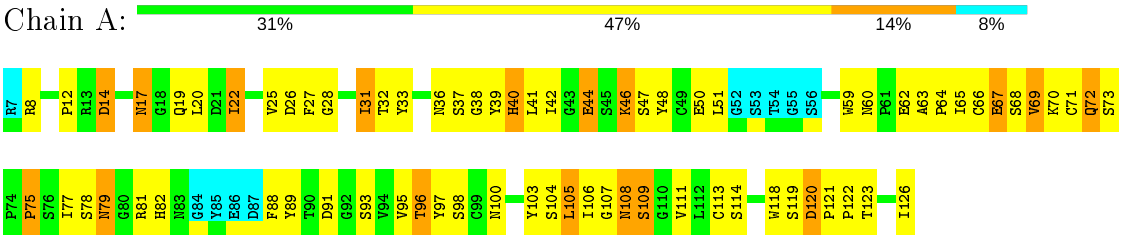
Chain A:



4.2.48 Score per residue for model 48

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

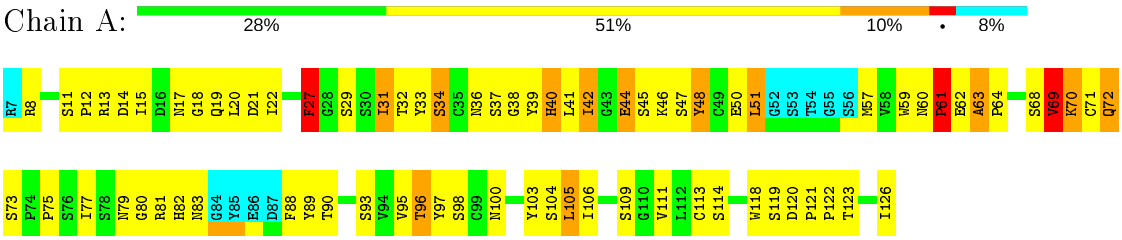
Chain A:



4.2.49 Score per residue for model 49

• Molecule 1: COMPLEMENT CONTROL PROTEIN C3

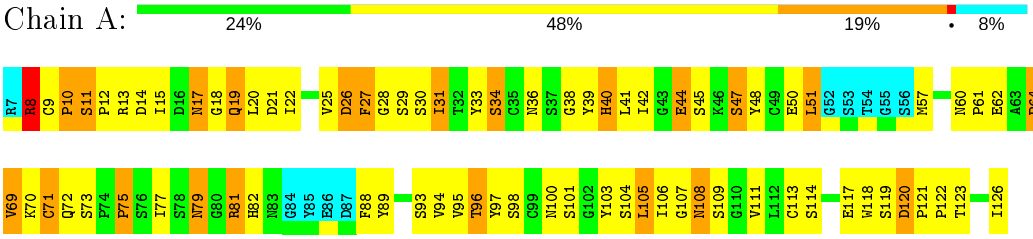
Chain A:



4.2.50 Score per residue for model 50

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3

Chain A:



5 Refinement protocol and experimental data overview

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

Of the ? calculated structures, 50 were deposited, based on the following criterion: *?*.

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

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

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

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.2
All	All	0	3

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	74	PRO	Mainchain	3

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	820	749	747	59±10
All	All	41000	37450	37352	2967

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 38.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:TYR:CE1	1:A:111:VAL:HG21	0.92	1.99	30	30
1:A:20:LEU:HD11	1:A:33:TYR:CZ	0.92	1.99	49	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:TYR:CE2	1:A:111:VAL:HG21	0.90	2.02	36	20
1:A:40:HIS:NE2	1:A:69:VAL:HG12	0.88	1.84	44	2
1:A:96:THR:HG22	1:A:109:SER:OG	0.87	1.69	23	36
1:A:41:LEU:HD21	1:A:44:GLU:O	0.86	1.70	34	46
1:A:20:LEU:HD11	1:A:33:TYR:CE2	0.85	2.06	1	15
1:A:40:HIS:CE1	1:A:42:ILE:HD11	0.85	2.07	24	38
1:A:112:LEU:HD22	1:A:113:CYS:N	0.84	1.87	38	13
1:A:13:ARG:O	1:A:20:LEU:HD21	0.84	1.72	15	22
1:A:15:ILE:HD13	1:A:33:TYR:CD2	0.84	2.07	20	1
1:A:20:LEU:HD22	1:A:33:TYR:CE1	0.83	2.08	24	6
1:A:20:LEU:HD11	1:A:33:TYR:CE1	0.82	2.09	50	11
1:A:14:ASP:O	1:A:20:LEU:HD21	0.81	1.74	46	1
1:A:74:PRO:HG2	1:A:95:VAL:HG21	0.80	1.53	6	2
1:A:27:PHE:CZ	1:A:51:LEU:HD23	0.80	2.11	44	5
1:A:38:GLY:O	1:A:69:VAL:HG22	0.80	1.76	26	28
1:A:20:LEU:HD22	1:A:33:TYR:CE2	0.80	2.12	22	8
1:A:19:GLN:C	1:A:20:LEU:HD13	0.78	1.99	21	2
1:A:22:ILE:HA	1:A:31:ILE:HG23	0.77	1.56	46	50
1:A:40:HIS:ND1	1:A:42:ILE:HD11	0.77	1.95	34	22
1:A:15:ILE:HD12	1:A:64:PRO:O	0.76	1.79	10	4
1:A:95:VAL:HG12	1:A:118:TRP:CH2	0.76	2.14	40	3
1:A:41:LEU:HD21	1:A:45:SER:CB	0.76	2.09	31	1
1:A:40:HIS:CE1	1:A:69:VAL:HG12	0.76	2.15	29	7
1:A:112:LEU:HD11	1:A:114:SER:HB2	0.75	1.59	6	7
1:A:20:LEU:HD21	1:A:33:TYR:CZ	0.74	2.17	29	4
1:A:41:LEU:C	1:A:42:ILE:HD13	0.74	2.02	6	9
1:A:20:LEU:HD13	1:A:33:TYR:CZ	0.74	2.17	16	2
1:A:77:ILE:HG22	1:A:122:PRO:O	0.74	1.82	30	2
1:A:31:ILE:HD11	1:A:59:TRP:CE3	0.73	2.18	17	29
1:A:41:LEU:HD11	1:A:64:PRO:HG2	0.73	1.61	33	33
1:A:96:THR:HG22	1:A:109:SER:HB2	0.72	1.59	30	10
1:A:74:PRO:CG	1:A:95:VAL:HG11	0.72	2.15	24	3
1:A:126:ILE:N	1:A:126:ILE:HD12	0.72	2.00	18	1
1:A:12:PRO:HG2	1:A:22:ILE:HD12	0.71	1.60	31	1
1:A:25:VAL:HG22	1:A:59:TRP:CZ2	0.71	2.20	29	2
1:A:41:LEU:HD21	1:A:64:PRO:HG2	0.71	1.61	49	4
1:A:13:ARG:O	1:A:20:LEU:HD11	0.70	1.87	11	10
1:A:14:ASP:O	1:A:63:ALA:HB2	0.69	1.87	30	6
1:A:20:LEU:HD23	1:A:20:LEU:N	0.69	2.02	11	8
1:A:74:PRO:CG	1:A:95:VAL:HG21	0.69	2.18	6	2
1:A:97:TYR:CZ	1:A:111:VAL:HG21	0.69	2.21	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:LEU:HD11	1:A:114:SER:OG	0.69	1.88	13	6
1:A:20:LEU:HD12	1:A:33:TYR:CE1	0.69	2.23	21	2
1:A:20:LEU:HD22	1:A:33:TYR:CD2	0.69	2.22	11	6
1:A:20:LEU:HD21	1:A:33:TYR:OH	0.69	1.87	2	4
1:A:12:PRO:HG2	1:A:22:ILE:HD13	0.68	1.64	48	6
1:A:105:LEU:HD12	1:A:124:CYS:SG	0.68	2.28	6	1
1:A:14:ASP:O	1:A:15:ILE:HG22	0.67	1.89	16	8
1:A:112:LEU:HD11	1:A:114:SER:HB3	0.67	1.66	31	2
1:A:112:LEU:HD11	1:A:114:SER:CB	0.67	2.20	31	12
1:A:20:LEU:HD22	1:A:20:LEU:N	0.66	2.05	31	1
1:A:8:ARG:HD2	1:A:25:VAL:HG23	0.66	1.68	26	7
1:A:38:GLY:O	1:A:69:VAL:HG13	0.66	1.91	29	3
1:A:41:LEU:O	1:A:41:LEU:HD23	0.66	1.91	29	1
1:A:74:PRO:HG3	1:A:95:VAL:HG11	0.65	1.66	40	3
1:A:51:LEU:O	1:A:58:VAL:HG22	0.65	1.90	46	2
1:A:20:LEU:N	1:A:20:LEU:HD22	0.65	2.06	46	3
1:A:22:ILE:HD13	1:A:31:ILE:HG21	0.65	1.69	31	1
1:A:106:ILE:HD11	1:A:125:GLN:HB2	0.65	1.69	8	3
1:A:12:PRO:HG3	1:A:22:ILE:HD13	0.65	1.68	30	3
1:A:12:PRO:CG	1:A:22:ILE:HD13	0.65	2.22	30	4
1:A:15:ILE:HD11	1:A:20:LEU:HD12	0.64	1.69	20	1
1:A:83:ASN:O	1:A:95:VAL:HG23	0.64	1.92	40	1
1:A:74:PRO:HG3	1:A:118:TRP:CE2	0.64	2.28	47	3
1:A:57:MET:O	1:A:58:VAL:HG13	0.64	1.92	24	7
1:A:33:TYR:CZ	1:A:62:GLU:O	0.63	2.51	10	9
1:A:42:ILE:N	1:A:42:ILE:HD13	0.63	2.08	6	4
1:A:77:ILE:HD11	1:A:80:GLY:HA3	0.63	1.69	47	4
1:A:14:ASP:C	1:A:20:LEU:HD11	0.63	2.14	21	1
1:A:69:VAL:HG22	1:A:116:GLY:HA3	0.62	1.71	17	3
1:A:63:ALA:HB1	1:A:64:PRO:CA	0.62	2.25	12	3
1:A:63:ALA:CB	1:A:64:PRO:HA	0.62	2.24	12	3
1:A:20:LEU:HD22	1:A:33:TYR:CD1	0.62	2.30	24	3
1:A:15:ILE:HG22	1:A:20:LEU:CD2	0.62	2.25	24	4
1:A:70:LYS:HE2	1:A:90:THR:HG23	0.61	1.71	49	3
1:A:112:LEU:HD22	1:A:113:CYS:H	0.61	1.55	38	12
1:A:126:ILE:HG22	1:A:126:ILE:O	0.61	1.95	33	12
1:A:33:TYR:O	1:A:41:LEU:HD13	0.61	1.96	26	2
1:A:69:VAL:HG23	1:A:69:VAL:O	0.61	1.96	13	9
1:A:22:ILE:HD13	1:A:31:ILE:HD13	0.61	1.71	25	1
1:A:41:LEU:HD11	1:A:64:PRO:CG	0.60	2.26	29	4
1:A:70:LYS:CE	1:A:90:THR:HG23	0.60	2.26	49	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LEU:HD21	1:A:64:PRO:HB2	0.60	1.71	41	1
1:A:31:ILE:HD11	1:A:59:TRP:CZ3	0.60	2.31	10	27
1:A:58:VAL:HG13	1:A:59:TRP:N	0.60	2.12	4	2
1:A:126:ILE:O	1:A:126:ILE:HG22	0.60	1.95	41	14
1:A:77:ILE:HG21	1:A:122:PRO:O	0.60	1.97	41	23
1:A:20:LEU:HD13	1:A:33:TYR:CE1	0.60	2.31	16	2
1:A:69:VAL:HG23	1:A:91:ASP:OD2	0.60	1.97	19	2
1:A:12:PRO:HB3	1:A:31:ILE:HD11	0.60	1.73	25	5
1:A:22:ILE:HD13	1:A:31:ILE:CG2	0.60	2.26	31	3
1:A:69:VAL:O	1:A:69:VAL:HG23	0.59	1.98	5	8
1:A:25:VAL:HG22	1:A:59:TRP:HZ2	0.59	1.57	27	2
1:A:19:GLN:C	1:A:20:LEU:HD22	0.59	2.18	46	1
1:A:63:ALA:HB1	1:A:64:PRO:HA	0.58	1.73	12	2
1:A:15:ILE:HG22	1:A:20:LEU:CD1	0.58	2.28	19	8
1:A:27:PHE:CZ	1:A:51:LEU:HD12	0.58	2.34	31	7
1:A:75:PRO:CB	1:A:97:TYR:CE1	0.58	2.87	47	2
1:A:73:SER:HG	1:A:82:HIS:CE1	0.58	2.17	11	11
1:A:32:THR:HG23	1:A:46:LYS:HG2	0.58	1.75	33	2
1:A:14:ASP:O	1:A:20:LEU:HD13	0.58	1.98	40	1
1:A:8:ARG:HD3	1:A:25:VAL:HG23	0.58	1.74	21	5
1:A:40:HIS:HB3	1:A:69:VAL:HG12	0.58	1.76	35	4
1:A:95:VAL:HG23	1:A:118:TRP:CH2	0.57	2.34	27	43
1:A:63:ALA:HB3	1:A:64:PRO:CA	0.57	2.28	6	1
1:A:120:ASP:N	1:A:121:PRO:CD	0.57	2.66	6	45
1:A:20:LEU:N	1:A:20:LEU:HD23	0.57	2.15	38	3
1:A:20:LEU:HD13	1:A:20:LEU:N	0.57	2.14	35	1
1:A:69:VAL:HG13	1:A:116:GLY:N	0.57	2.14	8	1
1:A:106:ILE:HD11	1:A:125:GLN:CG	0.57	2.29	24	1
1:A:112:LEU:HD13	1:A:112:LEU:C	0.57	2.20	37	7
1:A:20:LEU:H	1:A:20:LEU:HD22	0.56	1.60	21	2
1:A:75:PRO:CB	1:A:97:TYR:CE2	0.56	2.88	2	1
1:A:15:ILE:HG22	1:A:20:LEU:HD21	0.56	1.76	10	3
1:A:14:ASP:HA	1:A:20:LEU:HD11	0.56	1.77	25	5
1:A:51:LEU:C	1:A:51:LEU:HD12	0.56	2.21	35	3
1:A:111:VAL:HG13	1:A:119:SER:O	0.56	2.01	23	6
1:A:112:LEU:C	1:A:112:LEU:HD13	0.56	2.21	14	6
1:A:105:LEU:HD22	1:A:109:SER:HB2	0.56	1.77	33	4
1:A:20:LEU:N	1:A:20:LEU:HD13	0.56	2.16	21	1
1:A:41:LEU:C	1:A:41:LEU:HD23	0.56	2.21	1	15
1:A:31:ILE:CG1	1:A:59:TRP:CZ3	0.56	2.89	23	49
1:A:63:ALA:CB	1:A:64:PRO:CA	0.56	2.84	49	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:PHE:HZ	1:A:51:LEU:HD23	0.56	1.61	21	3
1:A:40:HIS:HB3	1:A:69:VAL:HG13	0.56	1.78	32	3
1:A:51:LEU:HD12	1:A:51:LEU:C	0.56	2.22	13	2
1:A:27:PHE:CE2	1:A:51:LEU:HD23	0.56	2.35	12	2
1:A:41:LEU:HD21	1:A:45:SER:HB3	0.55	1.78	31	1
1:A:95:VAL:CG1	1:A:118:TRP:CH2	0.55	2.90	8	3
1:A:105:LEU:HD11	1:A:109:SER:OG	0.55	2.02	7	2
1:A:27:PHE:CE1	1:A:57:MET:HE3	0.55	2.36	4	1
1:A:97:TYR:CE2	1:A:111:VAL:CG2	0.55	2.90	47	14
1:A:33:TYR:CE2	1:A:63:ALA:CA	0.55	2.90	6	1
1:A:48:TYR:CD2	1:A:48:TYR:N	0.55	2.73	49	2
1:A:41:LEU:HD21	1:A:45:SER:HB2	0.54	1.80	31	1
1:A:22:ILE:CA	1:A:31:ILE:HG23	0.54	2.31	46	15
1:A:41:LEU:HD12	1:A:66:CYS:SG	0.54	2.42	12	1
1:A:120:ASP:CB	1:A:121:PRO:CA	0.54	2.86	42	3
1:A:20:LEU:CD2	1:A:33:TYR:CZ	0.54	2.91	29	3
1:A:97:TYR:CD1	1:A:111:VAL:HG21	0.54	2.37	3	10
1:A:41:LEU:HD11	1:A:64:PRO:HD2	0.54	1.80	10	1
1:A:41:LEU:HD11	1:A:64:PRO:HG3	0.54	1.80	29	1
1:A:97:TYR:CE1	1:A:111:VAL:CG2	0.54	2.90	2	22
1:A:74:PRO:HG2	1:A:95:VAL:HG11	0.54	1.80	24	2
1:A:40:HIS:CE1	1:A:69:VAL:CG1	0.53	2.91	42	5
1:A:33:TYR:CE1	1:A:63:ALA:CB	0.53	2.91	40	5
1:A:20:LEU:CD1	1:A:33:TYR:CE1	0.53	2.91	12	9
1:A:39:TYR:CE1	1:A:68:SER:CB	0.53	2.92	31	14
1:A:58:VAL:CG1	1:A:59:TRP:N	0.53	2.71	28	2
1:A:41:LEU:HD23	1:A:41:LEU:C	0.53	2.24	4	11
1:A:103:TYR:CE2	1:A:126:ILE:CD1	0.53	2.91	6	1
1:A:20:LEU:CD2	1:A:33:TYR:CE2	0.53	2.91	25	8
1:A:105:LEU:HD22	1:A:109:SER:HB3	0.53	1.78	20	2
1:A:39:TYR:CE2	1:A:68:SER:CB	0.53	2.92	20	3
1:A:20:LEU:CD1	1:A:33:TYR:CE2	0.53	2.92	46	13
1:A:20:LEU:CD2	1:A:33:TYR:CE1	0.53	2.92	28	2
1:A:95:VAL:CG2	1:A:118:TRP:CH2	0.53	2.92	44	44
1:A:27:PHE:CZ	1:A:51:LEU:CD1	0.53	2.92	24	7
1:A:98:SER:HA	1:A:105:LEU:HD13	0.53	1.80	8	2
1:A:65:ILE:HD13	1:A:65:ILE:N	0.53	2.18	10	1
1:A:15:ILE:HD12	1:A:64:PRO:HD2	0.53	1.81	1	4
1:A:39:TYR:CZ	1:A:68:SER:CB	0.53	2.92	29	3
1:A:105:LEU:HD21	1:A:122:PRO:HG2	0.53	1.79	19	1
1:A:96:THR:HG22	1:A:109:SER:HG	0.53	1.64	21	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LEU:HD22	1:A:33:TYR:CZ	0.53	2.39	22	2
1:A:33:TYR:CE2	1:A:63:ALA:CB	0.52	2.92	9	4
1:A:105:LEU:HD11	1:A:109:SER:CB	0.52	2.34	7	2
1:A:17:ASN:CB	1:A:39:TYR:CE1	0.52	2.92	10	1
1:A:42:ILE:HB	1:A:65:ILE:HD12	0.52	1.81	20	4
1:A:120:ASP:HB3	1:A:121:PRO:CA	0.52	2.35	34	3
1:A:14:ASP:HA	1:A:20:LEU:HD21	0.52	1.81	21	1
1:A:106:ILE:HD11	1:A:125:GLN:HG3	0.52	1.79	24	1
1:A:105:LEU:HD12	1:A:109:SER:CA	0.52	2.34	48	2
1:A:42:ILE:HD13	1:A:42:ILE:N	0.52	2.19	25	6
1:A:95:VAL:HG23	1:A:118:TRP:CZ3	0.52	2.38	42	26
1:A:95:VAL:HG12	1:A:118:TRP:CZ3	0.52	2.40	40	3
1:A:77:ILE:HG23	1:A:97:TYR:HE2	0.52	1.65	23	16
1:A:40:HIS:CE1	1:A:42:ILE:CD1	0.52	2.92	14	33
1:A:27:PHE:CE1	1:A:57:MET:CE	0.52	2.93	4	1
1:A:12:PRO:CG	1:A:22:ILE:HD12	0.52	2.34	31	2
1:A:32:THR:HG23	1:A:46:LYS:CG	0.52	2.35	33	2
1:A:33:TYR:CE2	1:A:63:ALA:HA	0.52	2.39	49	12
1:A:126:ILE:CD1	1:A:126:ILE:N	0.52	2.71	18	1
1:A:103:TYR:CD1	1:A:126:ILE:CD1	0.52	2.92	41	2
1:A:112:LEU:HD21	1:A:114:SER:OG	0.52	2.04	1	3
1:A:70:LYS:CD	1:A:88:PHE:CD2	0.52	2.92	37	1
1:A:13:ARG:O	1:A:20:LEU:HD22	0.52	2.04	40	2
1:A:105:LEU:HD13	1:A:122:PRO:HB2	0.52	1.81	45	8
1:A:9:CYS:SG	1:A:49:CYS:CB	0.52	2.98	25	1
1:A:41:LEU:HD23	1:A:41:LEU:O	0.51	2.06	4	2
1:A:20:LEU:CG	1:A:33:TYR:CE1	0.51	2.92	40	2
1:A:25:VAL:HG12	1:A:59:TRP:CZ2	0.51	2.40	48	2
1:A:33:TYR:CD1	1:A:62:GLU:O	0.51	2.64	22	20
1:A:69:VAL:HG21	1:A:115:GLY:HA2	0.51	1.83	31	3
1:A:22:ILE:CG2	1:A:25:VAL:HG13	0.51	2.36	25	2
1:A:74:PRO:HG3	1:A:118:TRP:CZ2	0.51	2.40	47	2
1:A:109:SER:O	1:A:111:VAL:HG23	0.51	2.05	27	3
1:A:50:GLU:CG	1:A:51:LEU:N	0.51	2.74	49	19
1:A:20:LEU:CD1	1:A:33:TYR:CZ	0.51	2.93	16	2
1:A:33:TYR:CD2	1:A:62:GLU:O	0.51	2.64	29	13
1:A:32:THR:HG23	1:A:46:LYS:HD3	0.51	1.82	31	1
1:A:13:ARG:NH1	1:A:63:ALA:HB3	0.51	2.21	36	1
1:A:120:ASP:CB	1:A:121:PRO:HA	0.51	2.36	19	3
1:A:33:TYR:CG	1:A:62:GLU:O	0.51	2.64	21	7
1:A:33:TYR:CE2	1:A:63:ALA:HB1	0.51	2.41	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:ALA:HB3	1:A:64:PRO:HA	0.51	1.80	6	2
1:A:77:ILE:HG23	1:A:97:TYR:HE1	0.51	1.66	44	10
1:A:12:PRO:CG	1:A:31:ILE:HD13	0.51	2.36	50	1
1:A:48:TYR:CD1	1:A:60:ASN:CB	0.50	2.95	30	3
1:A:33:TYR:CG	1:A:63:ALA:O	0.50	2.64	6	2
1:A:69:VAL:HG21	1:A:91:ASP:OD2	0.50	2.06	22	1
1:A:39:TYR:CD1	1:A:68:SER:HA	0.50	2.42	8	14
1:A:12:PRO:CG	1:A:22:ILE:CD1	0.50	2.90	21	4
1:A:106:ILE:HG22	1:A:107:GLY:N	0.50	2.22	27	22
1:A:33:TYR:CD1	1:A:63:ALA:O	0.49	2.65	6	2
1:A:103:TYR:CZ	1:A:126:ILE:HD11	0.49	2.42	6	1
1:A:20:LEU:HD12	1:A:33:TYR:CD1	0.49	2.41	21	2
1:A:20:LEU:HD12	1:A:33:TYR:CZ	0.49	2.42	31	2
1:A:41:LEU:O	1:A:42:ILE:HD13	0.49	2.07	33	1
1:A:12:PRO:HG3	1:A:31:ILE:HD13	0.49	1.83	50	1
1:A:69:VAL:O	1:A:69:VAL:HG12	0.49	2.07	8	1
1:A:33:TYR:CE2	1:A:62:GLU:O	0.49	2.65	12	9
1:A:69:VAL:O	1:A:69:VAL:HG13	0.49	2.08	40	3
1:A:70:LYS:HG2	1:A:88:PHE:CD1	0.49	2.43	46	1
1:A:51:LEU:O	1:A:51:LEU:HD12	0.49	2.07	44	2
1:A:70:LYS:CG	1:A:88:PHE:CD1	0.49	2.96	46	1
1:A:119:SER:O	1:A:120:ASP:CB	0.49	2.61	19	3
1:A:9:CYS:HB3	1:A:10:PRO:CD	0.49	2.38	45	10
1:A:77:ILE:HG23	1:A:97:TYR:CE2	0.48	2.43	45	10
1:A:20:LEU:CD2	1:A:20:LEU:N	0.48	2.74	16	5
1:A:39:TYR:CG	1:A:67:GLU:O	0.48	2.67	10	20
1:A:97:TYR:CD2	1:A:111:VAL:HG21	0.48	2.43	36	6
1:A:20:LEU:N	1:A:20:LEU:CD2	0.48	2.75	46	1
1:A:73:SER:OG	1:A:82:HIS:CE1	0.48	2.67	7	23
1:A:33:TYR:CD2	1:A:63:ALA:O	0.48	2.67	6	3
1:A:12:PRO:CB	1:A:31:ILE:CD1	0.48	2.92	25	4
1:A:83:ASN:OD1	1:A:95:VAL:HG12	0.48	2.08	2	1
1:A:33:TYR:CE1	1:A:62:GLU:O	0.48	2.67	22	9
1:A:62:GLU:O	1:A:63:ALA:O	0.48	2.32	10	3
1:A:105:LEU:HD21	1:A:109:SER:HA	0.48	1.86	31	1
1:A:74:PRO:O	1:A:82:HIS:CE1	0.48	2.67	26	7
1:A:14:ASP:O	1:A:15:ILE:CG2	0.48	2.62	46	6
1:A:111:VAL:HG22	1:A:122:PRO:HD3	0.48	1.84	27	3
1:A:69:VAL:HG22	1:A:91:ASP:HB3	0.48	1.84	2	1
1:A:106:ILE:O	1:A:122:PRO:CB	0.48	2.62	7	49
1:A:39:TYR:CD1	1:A:67:GLU:O	0.48	2.66	36	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:THR:HG22	1:A:125:GLN:HE22	0.48	1.67	21	2
1:A:40:HIS:CD2	1:A:40:HIS:O	0.48	2.67	19	6
1:A:74:PRO:CG	1:A:118:TRP:CZ2	0.48	2.96	47	2
1:A:39:TYR:CD2	1:A:67:GLU:O	0.48	2.67	42	6
1:A:39:TYR:CZ	1:A:68:SER:HB3	0.48	2.44	9	10
1:A:22:ILE:CG2	1:A:25:VAL:CG1	0.48	2.91	25	2
1:A:20:LEU:HD21	1:A:33:TYR:CE1	0.48	2.43	40	1
1:A:80:GLY:N	1:A:100:ASN:ND2	0.48	2.62	13	25
1:A:77:ILE:HG23	1:A:97:TYR:CE1	0.48	2.44	10	4
1:A:48:TYR:CE1	1:A:61:PRO:HD3	0.48	2.44	44	4
1:A:97:TYR:HB2	1:A:105:LEU:HD11	0.48	1.85	30	2
1:A:33:TYR:CE1	1:A:63:ALA:HA	0.48	2.43	10	7
1:A:14:ASP:C	1:A:20:LEU:HD21	0.48	2.27	46	3
1:A:47:SER:HA	1:A:61:PRO:O	0.48	2.08	49	4
1:A:105:LEU:HD11	1:A:122:PRO:HG2	0.48	1.86	34	1
1:A:47:SER:CB	1:A:61:PRO:O	0.47	2.62	12	1
1:A:41:LEU:CD1	1:A:65:ILE:O	0.47	2.62	31	1
1:A:9:CYS:O	1:A:10:PRO:O	0.47	2.31	50	1
1:A:22:ILE:CD1	1:A:31:ILE:HD13	0.47	2.39	25	1
1:A:120:ASP:HB3	1:A:121:PRO:HA	0.47	1.86	34	2
1:A:20:LEU:CD1	1:A:20:LEU:N	0.47	2.77	15	2
1:A:74:PRO:O	1:A:82:HIS:CD2	0.47	2.67	30	3
1:A:31:ILE:HD12	1:A:47:SER:HB2	0.47	1.86	49	1
1:A:79:ASN:ND2	1:A:79:ASN:N	0.47	2.63	23	7
1:A:72:GLN:CG	1:A:73:SER:N	0.47	2.77	36	7
1:A:48:TYR:CD1	1:A:60:ASN:O	0.47	2.67	44	3
1:A:40:HIS:O	1:A:40:HIS:CD2	0.47	2.68	15	9
1:A:75:PRO:HB3	1:A:97:TYR:CE2	0.47	2.43	2	1
1:A:39:TYR:CE1	1:A:68:SER:HB3	0.47	2.45	16	13
1:A:88:PHE:C	1:A:89:TYR:CD2	0.47	2.88	19	24
1:A:83:ASN:CB	1:A:96:THR:O	0.47	2.62	6	1
1:A:31:ILE:HG12	1:A:59:TRP:CZ3	0.47	2.44	14	10
1:A:33:TYR:CG	1:A:64:PRO:CD	0.47	2.98	26	1
1:A:40:HIS:CG	1:A:42:ILE:HD11	0.47	2.44	34	1
1:A:70:LYS:CD	1:A:88:PHE:CG	0.47	2.98	37	1
1:A:41:LEU:HD22	1:A:45:SER:HB3	0.47	1.87	44	1
1:A:40:HIS:CG	1:A:40:HIS:O	0.47	2.67	31	8
1:A:105:LEU:HD22	1:A:109:SER:CB	0.47	2.39	20	3
1:A:88:PHE:C	1:A:89:TYR:CD1	0.47	2.89	27	23
1:A:83:ASN:N	1:A:96:THR:O	0.47	2.47	6	3
1:A:94:VAL:HG12	1:A:95:VAL:N	0.47	2.25	13	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:LYS:HA	1:A:89:TYR:O	0.47	2.10	37	1
1:A:31:ILE:HD12	1:A:47:SER:CB	0.47	2.40	49	2
1:A:48:TYR:CD1	1:A:60:ASN:HB3	0.47	2.45	21	18
1:A:20:LEU:N	1:A:20:LEU:HD12	0.47	2.25	15	2
1:A:70:LYS:HD3	1:A:88:PHE:CD2	0.46	2.46	37	1
1:A:105:LEU:HD21	1:A:122:PRO:CG	0.46	2.40	23	3
1:A:79:ASN:N	1:A:79:ASN:ND2	0.46	2.63	19	5
1:A:17:ASN:HB3	1:A:39:TYR:CE1	0.46	2.45	10	5
1:A:75:PRO:O	1:A:76:SER:CB	0.46	2.63	30	1
1:A:112:LEU:HD12	1:A:119:SER:OG	0.46	2.09	42	1
1:A:27:PHE:HZ	1:A:51:LEU:HD12	0.46	1.69	6	3
1:A:97:TYR:CB	1:A:105:LEU:HD11	0.46	2.40	48	2
1:A:17:ASN:ND2	1:A:17:ASN:N	0.46	2.63	16	10
1:A:41:LEU:CD2	1:A:44:GLU:O	0.46	2.64	12	4
1:A:103:TYR:CZ	1:A:126:ILE:HG12	0.46	2.46	33	1
1:A:42:ILE:O	1:A:64:PRO:CB	0.46	2.64	10	3
1:A:47:SER:OG	1:A:62:GLU:CB	0.46	2.64	4	14
1:A:48:TYR:CD2	1:A:60:ASN:HB3	0.46	2.46	38	7
1:A:27:PHE:HZ	1:A:51:LEU:HD22	0.46	1.70	37	4
1:A:33:TYR:CE1	1:A:63:ALA:HB2	0.46	2.46	43	4
1:A:111:VAL:HG12	1:A:118:TRP:CE3	0.46	2.46	27	2
1:A:75:PRO:HB3	1:A:97:TYR:CE1	0.46	2.45	47	1
1:A:39:TYR:CE1	1:A:68:SER:HB2	0.46	2.46	37	6
1:A:27:PHE:CZ	1:A:51:LEU:HD22	0.46	2.46	8	7
1:A:39:TYR:CE2	1:A:68:SER:HB3	0.46	2.45	29	8
1:A:60:ASN:CB	1:A:61:PRO:HD2	0.46	2.41	49	14
1:A:103:TYR:CE1	1:A:126:ILE:HG12	0.46	2.46	32	11
1:A:13:ARG:O	1:A:20:LEU:CD2	0.46	2.64	20	8
1:A:9:CYS:CB	1:A:59:TRP:NE1	0.46	2.79	39	2
1:A:41:LEU:HD13	1:A:45:SER:OG	0.46	2.11	23	1
1:A:39:TYR:CD2	1:A:68:SER:HA	0.46	2.46	46	7
1:A:63:ALA:HB1	1:A:64:PRO:C	0.46	2.31	10	3
1:A:17:ASN:N	1:A:17:ASN:ND2	0.46	2.64	12	6
1:A:82:HIS:HB3	1:A:97:TYR:CE1	0.46	2.46	22	2
1:A:15:ILE:CD1	1:A:33:TYR:CD2	0.46	2.91	20	1
1:A:81:ARG:N	1:A:98:SER:O	0.45	2.49	30	21
1:A:15:ILE:HG12	1:A:33:TYR:CE2	0.45	2.46	20	1
1:A:62:GLU:O	1:A:64:PRO:HD2	0.45	2.11	31	5
1:A:103:TYR:CD2	1:A:126:ILE:CD1	0.45	2.99	1	2
1:A:40:HIS:ND1	1:A:42:ILE:CD1	0.45	2.78	3	8
1:A:107:GLY:O	1:A:108:ASN:ND2	0.45	2.49	36	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:TYR:CE2	1:A:68:SER:OG	0.45	2.69	20	1
1:A:62:GLU:O	1:A:64:PRO:CD	0.45	2.64	29	7
1:A:25:VAL:O	1:A:25:VAL:CG1	0.45	2.64	29	1
1:A:74:PRO:HD2	1:A:89:TYR:CE2	0.45	2.46	47	1
1:A:70:LYS:CE	1:A:90:THR:CG2	0.45	2.94	49	1
1:A:103:TYR:CE2	1:A:126:ILE:HG12	0.45	2.45	11	27
1:A:15:ILE:HD11	1:A:66:CYS:HB2	0.45	1.87	6	1
1:A:77:ILE:CG2	1:A:122:PRO:O	0.45	2.65	27	6
1:A:13:ARG:O	1:A:20:LEU:CD1	0.45	2.64	16	11
1:A:105:LEU:HD22	1:A:109:SER:CA	0.45	2.42	21	1
1:A:106:ILE:CG1	1:A:125:GLN:HG2	0.45	2.41	24	1
1:A:112:LEU:C	1:A:112:LEU:HD22	0.45	2.32	31	1
1:A:89:TYR:CE2	1:A:95:VAL:CG1	0.45	3.00	6	1
1:A:70:LYS:HZ1	1:A:72:GLN:HA	0.45	1.70	37	1
1:A:70:LYS:HD2	1:A:88:PHE:CG	0.45	2.47	37	1
1:A:17:ASN:HB3	1:A:39:TYR:CE2	0.45	2.47	18	7
1:A:33:TYR:CE2	1:A:63:ALA:C	0.45	2.90	6	1
1:A:74:PRO:HB2	1:A:82:HIS:CG	0.45	2.47	27	3
1:A:120:ASP:N	1:A:121:PRO:HD3	0.45	2.27	10	20
1:A:97:TYR:CD2	1:A:122:PRO:HG2	0.45	2.47	50	5
1:A:40:HIS:CE1	1:A:42:ILE:HD12	0.45	2.46	12	1
1:A:68:SER:OG	1:A:90:THR:HG22	0.45	2.12	25	2
1:A:71:CYS:N	1:A:89:TYR:O	0.45	2.50	38	8
1:A:33:TYR:CD2	1:A:63:ALA:C	0.45	2.90	6	2
1:A:33:TYR:CE1	1:A:63:ALA:O	0.45	2.70	6	1
1:A:10:PRO:HD2	1:A:59:TRP:CD1	0.45	2.47	2	10
1:A:88:PHE:O	1:A:89:TYR:CG	0.45	2.70	46	2
1:A:75:PRO:HD3	1:A:118:TRP:CG	0.45	2.47	50	20
1:A:33:TYR:CE1	1:A:62:GLU:C	0.45	2.91	36	3
1:A:40:HIS:O	1:A:40:HIS:CG	0.45	2.70	1	10
1:A:105:LEU:HD11	1:A:109:SER:CA	0.45	2.42	3	2
1:A:97:TYR:CD1	1:A:122:PRO:HD2	0.45	2.47	6	1
1:A:39:TYR:CE2	1:A:68:SER:HB2	0.45	2.46	36	4
1:A:79:ASN:HB3	1:A:103:TYR:CD1	0.44	2.47	34	18
1:A:25:VAL:CG1	1:A:25:VAL:O	0.44	2.65	27	1
1:A:44:GLU:O	1:A:64:PRO:CG	0.44	2.65	44	27
1:A:40:HIS:N	1:A:40:HIS:CD2	0.44	2.86	42	3
1:A:20:LEU:HG	1:A:33:TYR:CE1	0.44	2.48	49	3
1:A:70:LYS:HG2	1:A:88:PHE:CD2	0.44	2.47	19	1
1:A:65:ILE:HG22	1:A:66:CYS:H	0.44	1.72	43	7
1:A:63:ALA:O	1:A:64:PRO:O	0.44	2.36	31	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ILE:HG23	1:A:18:GLY:C	0.44	2.32	50	4
1:A:31:ILE:CD1	1:A:47:SER:OG	0.44	2.66	50	1
1:A:50:GLU:O	1:A:58:VAL:N	0.44	2.50	13	1
1:A:71:CYS:O	1:A:89:TYR:N	0.44	2.51	35	23
1:A:69:VAL:HG13	1:A:116:GLY:H	0.44	1.72	8	1
1:A:49:CYS:HB3	1:A:59:TRP:CD2	0.44	2.47	25	1
1:A:97:TYR:HE1	1:A:111:VAL:HG21	0.44	1.66	29	1
1:A:69:VAL:HB	1:A:116:GLY:N	0.44	2.27	46	4
1:A:105:LEU:CD1	1:A:109:SER:CA	0.44	2.95	7	2
1:A:50:GLU:HG2	1:A:51:LEU:N	0.44	2.27	14	11
1:A:111:VAL:CG1	1:A:118:TRP:HB3	0.44	2.42	27	3
1:A:18:GLY:CA	1:A:34:SER:O	0.44	2.66	47	19
1:A:60:ASN:O	1:A:61:PRO:O	0.44	2.36	49	2
1:A:14:ASP:O	1:A:15:ILE:O	0.44	2.36	34	3
1:A:33:TYR:CG	1:A:64:PRO:HD2	0.44	2.47	26	1
1:A:21:ASP:N	1:A:32:THR:O	0.44	2.51	34	19
1:A:33:TYR:CE2	1:A:62:GLU:CB	0.44	3.01	7	1
1:A:12:PRO:HG2	1:A:22:ILE:CD1	0.44	2.43	35	1
1:A:104:SER:CB	1:A:125:GLN:O	0.44	2.66	6	4
1:A:48:TYR:CD2	1:A:60:ASN:CB	0.44	3.00	36	5
1:A:83:ASN:OD1	1:A:95:VAL:CG1	0.44	2.66	5	2
1:A:33:TYR:CD1	1:A:64:PRO:HD3	0.44	2.47	33	3
1:A:105:LEU:HD12	1:A:109:SER:HA	0.44	1.90	22	3
1:A:97:TYR:CD1	1:A:122:PRO:HG2	0.44	2.48	38	1
1:A:107:GLY:O	1:A:108:ASN:O	0.43	2.35	36	5
1:A:48:TYR:HB2	1:A:60:ASN:HB2	0.43	1.90	4	7
1:A:19:GLN:N	1:A:34:SER:O	0.43	2.51	29	12
1:A:60:ASN:O	1:A:61:PRO:C	0.43	2.57	10	5
1:A:103:TYR:HA	1:A:126:ILE:HD13	0.43	1.90	46	1
1:A:94:VAL:CG1	1:A:95:VAL:N	0.43	2.80	13	8
1:A:74:PRO:HD2	1:A:89:TYR:CE1	0.43	2.47	27	1
1:A:68:SER:OG	1:A:90:THR:CG2	0.43	2.66	33	1
1:A:27:PHE:CE2	1:A:51:LEU:HG	0.43	2.48	46	1
1:A:51:LEU:C	1:A:58:VAL:HG22	0.43	2.33	31	2
1:A:123:THR:HG22	1:A:125:GLN:NE2	0.43	2.28	21	1
1:A:33:TYR:CE2	1:A:62:GLU:C	0.43	2.92	35	4
1:A:44:GLU:O	1:A:64:PRO:CB	0.43	2.67	33	9
1:A:44:GLU:O	1:A:64:PRO:HG3	0.43	2.13	6	1
1:A:51:LEU:O	1:A:58:VAL:CG2	0.43	2.66	11	1
1:A:70:LYS:CD	1:A:88:PHE:HB3	0.43	2.44	19	2
1:A:69:VAL:O	1:A:116:GLY:N	0.43	2.52	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:TYR:CD2	1:A:111:VAL:CG2	0.43	3.01	34	3
1:A:20:LEU:CG	1:A:33:TYR:CZ	0.43	3.02	2	1
1:A:106:ILE:CG2	1:A:107:GLY:N	0.43	2.82	47	5
1:A:20:LEU:HD12	1:A:33:TYR:CE2	0.43	2.48	31	1
1:A:41:LEU:CD1	1:A:64:PRO:HG2	0.43	2.44	31	1
1:A:88:PHE:O	1:A:89:TYR:CD1	0.43	2.72	46	1
1:A:47:SER:OG	1:A:62:GLU:CG	0.43	2.66	13	11
1:A:75:PRO:HD3	1:A:118:TRP:CD1	0.43	2.48	30	20
1:A:97:TYR:N	1:A:109:SER:OG	0.43	2.51	36	6
1:A:69:VAL:HG21	1:A:115:GLY:CA	0.43	2.44	6	2
1:A:12:PRO:HB3	1:A:31:ILE:HD13	0.43	1.90	14	1
1:A:79:ASN:HB3	1:A:103:TYR:CD2	0.43	2.49	22	6
1:A:88:PHE:O	1:A:89:TYR:CD2	0.43	2.71	19	1
1:A:27:PHE:CZ	1:A:51:LEU:HG	0.43	2.48	31	4
1:A:12:PRO:CB	1:A:31:ILE:HD11	0.43	2.43	25	1
1:A:33:TYR:OH	1:A:62:GLU:CB	0.43	2.67	4	4
1:A:113:CYS:HB2	1:A:118:TRP:CZ3	0.43	2.49	42	14
1:A:97:TYR:CD1	1:A:111:VAL:CG2	0.43	3.02	3	4
1:A:73:SER:OG	1:A:82:HIS:NE2	0.43	2.52	29	16
1:A:39:TYR:CB	1:A:67:GLU:O	0.43	2.67	23	4
1:A:13:ARG:CB	1:A:33:TYR:OH	0.43	2.67	29	2
1:A:105:LEU:HD23	1:A:122:PRO:HB2	0.43	1.89	21	1
1:A:49:CYS:SG	1:A:59:TRP:CH2	0.43	3.11	25	1
1:A:83:ASN:OD1	1:A:96:THR:N	0.43	2.52	40	1
1:A:63:ALA:HB3	1:A:64:PRO:C	0.43	2.34	6	1
1:A:26:ASP:O	1:A:28:GLY:N	0.43	2.52	16	11
1:A:123:THR:CG2	1:A:125:GLN:NE2	0.43	2.82	15	1
1:A:105:LEU:HA	1:A:124:CYS:HA	0.43	1.90	3	1
1:A:40:HIS:CD2	1:A:40:HIS:N	0.43	2.86	36	2
1:A:104:SER:O	1:A:125:GLN:N	0.43	2.51	6	1
1:A:70:LYS:CG	1:A:89:TYR:O	0.43	2.67	47	2
1:A:9:CYS:HB2	1:A:59:TRP:CZ2	0.43	2.48	25	1
1:A:14:ASP:O	1:A:63:ALA:CB	0.43	2.67	26	2
1:A:8:ARG:CD	1:A:25:VAL:HG12	0.43	2.43	27	1
1:A:77:ILE:HG13	1:A:78:SER:N	0.43	2.29	30	2
1:A:47:SER:C	1:A:48:TYR:CD2	0.43	2.92	44	2
1:A:105:LEU:CD1	1:A:122:PRO:HB2	0.43	2.44	44	4
1:A:76:SER:OG	1:A:77:ILE:N	0.43	2.52	30	1
1:A:105:LEU:HA	1:A:123:THR:O	0.42	2.14	3	2
1:A:39:TYR:CD2	1:A:67:GLU:C	0.42	2.92	15	6
1:A:83:ASN:ND2	1:A:96:THR:O	0.42	2.52	47	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:VAL:HG13	1:A:120:ASP:HB2	0.42	1.91	42	2
1:A:69:VAL:CG2	1:A:91:ASP:OD1	0.42	2.67	48	3
1:A:24:GLY:O	1:A:29:SER:CB	0.42	2.67	2	3
1:A:120:ASP:HB3	1:A:121:PRO:C	0.42	2.34	42	1
1:A:9:CYS:HB3	1:A:59:TRP:NE1	0.42	2.28	15	11
1:A:48:TYR:CD1	1:A:48:TYR:N	0.42	2.86	5	1
1:A:12:PRO:HB3	1:A:31:ILE:CD1	0.42	2.43	26	8
1:A:48:TYR:N	1:A:60:ASN:O	0.42	2.49	6	1
1:A:17:ASN:CB	1:A:39:TYR:CE2	0.42	3.02	34	2
1:A:8:ARG:HB3	1:A:25:VAL:HG23	0.42	1.91	46	1
1:A:70:LYS:HE3	1:A:90:THR:HG23	0.42	1.89	31	2
1:A:20:LEU:N	1:A:20:LEU:CD1	0.42	2.82	40	1
1:A:105:LEU:CD1	1:A:109:SER:HA	0.42	2.45	7	2
1:A:31:ILE:O	1:A:46:LYS:CG	0.42	2.68	4	8
1:A:28:GLY:N	1:A:49:CYS:O	0.42	2.53	43	4
1:A:20:LEU:HD11	1:A:33:TYR:CD2	0.42	2.49	6	1
1:A:33:TYR:CE2	1:A:63:ALA:O	0.42	2.73	6	1
1:A:40:HIS:CE1	1:A:69:VAL:HA	0.42	2.50	25	4
1:A:31:ILE:CD1	1:A:59:TRP:CZ3	0.42	3.00	10	3
1:A:31:ILE:N	1:A:47:SER:O	0.42	2.52	15	2
1:A:69:VAL:CG2	1:A:91:ASP:OD2	0.42	2.67	25	3
1:A:77:ILE:HD12	1:A:124:CYS:HB2	0.42	1.92	27	2
1:A:33:TYR:CE2	1:A:62:GLU:HB3	0.42	2.49	42	1
1:A:65:ILE:HG22	1:A:66:CYS:N	0.42	2.30	17	11
1:A:40:HIS:NE2	1:A:42:ILE:HD11	0.42	2.29	19	1
1:A:27:PHE:CE1	1:A:57:MET:SD	0.42	3.12	26	1
1:A:69:VAL:HG21	1:A:115:GLY:H	0.42	1.75	13	1
1:A:33:TYR:CZ	1:A:63:ALA:O	0.42	2.73	6	1
1:A:63:ALA:CB	1:A:64:PRO:O	0.42	2.67	6	1
1:A:97:TYR:N	1:A:109:SER:O	0.42	2.53	12	2
1:A:22:ILE:HG21	1:A:25:VAL:CG1	0.42	2.44	34	1
1:A:70:LYS:HE3	1:A:90:THR:CG2	0.42	2.45	49	1
1:A:75:PRO:N	1:A:97:TYR:OH	0.42	2.53	8	2
1:A:103:TYR:CD2	1:A:126:ILE:HG13	0.42	2.50	18	1
1:A:17:ASN:HB2	1:A:39:TYR:CD2	0.42	2.50	34	1
1:A:45:SER:O	1:A:46:LYS:CG	0.42	2.68	35	2
1:A:72:GLN:O	1:A:118:TRP:NE1	0.42	2.48	37	2
1:A:91:ASP:OD1	1:A:115:GLY:N	0.42	2.53	38	2
1:A:48:TYR:N	1:A:48:TYR:CD1	0.42	2.87	40	1
1:A:113:CYS:HB2	1:A:118:TRP:CH2	0.42	2.50	43	9
1:A:14:ASP:C	1:A:15:ILE:CG1	0.42	2.88	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:ARG:CG	1:A:98:SER:O	0.42	2.68	47	2
1:A:50:GLU:OE2	1:A:60:ASN:ND2	0.42	2.53	32	1
1:A:8:ARG:CB	1:A:25:VAL:O	0.42	2.68	41	1
1:A:106:ILE:O	1:A:122:PRO:CA	0.42	2.68	4	3
1:A:100:ASN:CG	1:A:101:SER:N	0.42	2.73	4	2
1:A:44:GLU:O	1:A:64:PRO:HG2	0.42	2.14	10	1
1:A:15:ILE:CD1	1:A:20:LEU:HD12	0.42	2.44	20	1
1:A:31:ILE:O	1:A:46:LYS:CD	0.42	2.67	38	2
1:A:27:PHE:CE1	1:A:50:GLU:HA	0.42	2.50	47	2
1:A:83:ASN:ND2	1:A:96:THR:OG1	0.42	2.53	30	3
1:A:68:SER:O	1:A:70:LYS:N	0.42	2.52	20	8
1:A:48:TYR:O	1:A:50:GLU:N	0.42	2.53	9	1
1:A:38:GLY:O	1:A:69:VAL:CG2	0.42	2.68	9	1
1:A:112:LEU:HD13	1:A:112:LEU:O	0.42	2.14	46	2
1:A:69:VAL:CG2	1:A:69:VAL:O	0.42	2.67	13	1
1:A:17:ASN:O	1:A:36:ASN:N	0.41	2.53	28	4
1:A:46:LYS:HB3	1:A:48:TYR:CE2	0.41	2.50	12	1
1:A:49:CYS:HB3	1:A:59:TRP:CE2	0.41	2.50	25	1
1:A:31:ILE:O	1:A:46:LYS:CE	0.41	2.68	40	1
1:A:11:SER:CB	1:A:12:PRO:C	0.41	2.89	50	1
1:A:11:SER:HG	1:A:12:PRO:C	0.41	2.19	50	1
1:A:31:ILE:HG13	1:A:59:TRP:CZ3	0.41	2.49	3	1
1:A:33:TYR:CZ	1:A:63:ALA:HA	0.41	2.50	26	3
1:A:33:TYR:N	1:A:45:SER:O	0.41	2.50	31	2
1:A:97:TYR:CD2	1:A:122:PRO:HD2	0.41	2.50	12	1
1:A:20:LEU:HD12	1:A:20:LEU:N	0.41	2.30	34	1
1:A:81:ARG:NE	1:A:100:ASN:OD1	0.41	2.53	41	1
1:A:40:HIS:N	1:A:67:GLU:O	0.41	2.52	48	1
1:A:44:GLU:OE2	1:A:61:PRO:CB	0.41	2.68	19	1
1:A:15:ILE:HG12	1:A:20:LEU:CD1	0.41	2.45	20	1
1:A:20:LEU:HG	1:A:33:TYR:CZ	0.41	2.49	2	1
1:A:75:PRO:CA	1:A:97:TYR:CE2	0.41	3.03	2	1
1:A:27:PHE:CZ	1:A:51:LEU:CD2	0.41	3.03	5	1
1:A:83:ASN:HB3	1:A:96:THR:O	0.41	2.16	6	1
1:A:70:LYS:CE	1:A:88:PHE:HB3	0.41	2.45	46	2
1:A:47:SER:CA	1:A:61:PRO:O	0.41	2.68	30	1
1:A:70:LYS:HD2	1:A:88:PHE:CD2	0.41	2.49	37	1
1:A:81:ARG:CD	1:A:100:ASN:OD1	0.41	2.68	49	2
1:A:75:PRO:HA	1:A:97:TYR:CZ	0.41	2.51	2	1
1:A:103:TYR:CB	1:A:124:CYS:SG	0.41	3.09	5	2
1:A:89:TYR:CB	1:A:113:CYS:SG	0.41	3.08	12	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:PHE:CZ	1:A:51:LEU:HB3	0.41	2.50	28	2
1:A:82:HIS:HB3	1:A:97:TYR:CE2	0.41	2.51	34	1
1:A:26:ASP:OD1	1:A:27:PHE:N	0.41	2.52	13	1
1:A:12:PRO:HG3	1:A:59:TRP:CZ2	0.41	2.51	40	3
1:A:41:LEU:CD2	1:A:45:SER:CB	0.41	2.94	31	1
1:A:74:PRO:O	1:A:82:HIS:ND1	0.41	2.54	2	1
1:A:48:TYR:CB	1:A:60:ASN:HB2	0.41	2.46	19	2
1:A:104:SER:N	1:A:125:GLN:O	0.41	2.53	46	2
1:A:26:ASP:N	1:A:29:SER:OG	0.41	2.53	42	2
1:A:12:PRO:HG3	1:A:31:ILE:CD1	0.41	2.45	50	1
1:A:16:ASP:O	1:A:18:GLY:N	0.41	2.54	4	2
1:A:42:ILE:O	1:A:64:PRO:HB2	0.41	2.16	12	2
1:A:15:ILE:CD1	1:A:64:PRO:O	0.41	2.68	12	1
1:A:39:TYR:CE2	1:A:67:GLU:HA	0.41	2.50	12	1
1:A:44:GLU:C	1:A:64:PRO:CG	0.41	2.89	49	2
1:A:91:ASP:OD2	1:A:91:ASP:N	0.41	2.54	19	1
1:A:15:ILE:HG23	1:A:33:TYR:CE2	0.41	2.51	20	1
1:A:39:TYR:CA	1:A:67:GLU:O	0.41	2.69	23	2
1:A:70:LYS:HD2	1:A:88:PHE:CD1	0.41	2.51	27	1
1:A:105:LEU:HD12	1:A:109:SER:CB	0.41	2.45	30	1
1:A:47:SER:OG	1:A:60:ASN:O	0.41	2.37	46	1
1:A:27:PHE:CE2	1:A:51:LEU:HB3	0.41	2.51	28	1
1:A:51:LEU:HD23	1:A:51:LEU:H	0.41	1.75	32	1
1:A:79:ASN:HB3	1:A:103:TYR:CE2	0.41	2.51	48	1
1:A:103:TYR:CD2	1:A:126:ILE:HG12	0.40	2.51	3	1
1:A:9:CYS:N	1:A:25:VAL:O	0.40	2.53	27	1
1:A:38:GLY:O	1:A:69:VAL:CG1	0.40	2.67	29	1
1:A:103:TYR:CD1	1:A:126:ILE:HG12	0.40	2.51	30	1
1:A:48:TYR:O	1:A:60:ASN:N	0.40	2.52	38	1
1:A:103:TYR:CE1	1:A:126:ILE:HD11	0.40	2.51	41	1
1:A:49:CYS:HB2	1:A:59:TRP:CH2	0.40	2.51	41	1
1:A:48:TYR:CE1	1:A:61:PRO:CD	0.40	3.04	44	1
1:A:33:TYR:CZ	1:A:63:ALA:HB2	0.40	2.51	9	1
1:A:48:TYR:CE2	1:A:61:PRO:HD3	0.40	2.51	17	1
1:A:15:ILE:HG23	1:A:33:TYR:CD2	0.40	2.50	20	1
1:A:97:TYR:CB	1:A:122:PRO:HG2	0.40	2.46	31	1
1:A:31:ILE:CD1	1:A:47:SER:HB3	0.40	2.46	35	1
1:A:79:ASN:HB3	1:A:103:TYR:CE1	0.40	2.51	50	1
1:A:47:SER:OG	1:A:62:GLU:CA	0.40	2.70	27	2
1:A:109:SER:HA	1:A:122:PRO:HG3	0.40	1.93	3	1
1:A:31:ILE:CG1	1:A:47:SER:HB2	0.40	2.47	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:TYR:CZ	1:A:68:SER:HB2	0.40	2.50	29	1
1:A:105:LEU:CD2	1:A:109:SER:HA	0.40	2.47	47	1
1:A:14:ASP:O	1:A:20:LEU:CD1	0.40	2.70	15	1
1:A:27:PHE:CE2	1:A:50:GLU:HA	0.40	2.51	17	1
1:A:33:TYR:CD2	1:A:63:ALA:HA	0.40	2.52	46	1
1:A:70:LYS:HD3	1:A:88:PHE:CG	0.40	2.52	46	1
1:A:75:PRO:CA	1:A:97:TYR:CE1	0.40	3.03	47	1
1:A:111:VAL:HG12	1:A:118:TRP:HE3	0.40	1.75	6	1
1:A:74:PRO:CG	1:A:95:VAL:CG1	0.40	2.96	8	1
1:A:47:SER:CB	1:A:62:GLU:OE1	0.40	2.69	22	1
1:A:74:PRO:CB	1:A:97:TYR:OH	0.40	2.69	30	1
1:A:70:LYS:CA	1:A:89:TYR:O	0.40	2.70	37	1
1:A:44:GLU:OE1	1:A:61:PRO:CG	0.40	2.69	43	1
1:A:75:PRO:HA	1:A:97:TYR:CE2	0.40	2.51	2	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	109/120 (91%)	80±2 (74±2%)	20±3 (19±3%)	8±2 (8±2%)	2	15
All	All	5450/6000 (91%)	4020 (74%)	1020 (19%)	410 (8%)	2	15

All 31 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	64	PRO	47
1	A	69	VAL	47
1	A	36	ASN	38
1	A	61	PRO	36
1	A	27	PHE	35
1	A	75	PRO	34
1	A	72	GLN	31
1	A	91	ASP	23

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Mol	Chain	Res	Type	Models (Total)
1	A	108	ASN	18
1	A	8	ARG	16
1	A	45	SER	15
1	A	15	ILE	9
1	A	13	ARG	8
1	A	12	PRO	7
1	A	44	GLU	7
1	A	102	GLY	6
1	A	74	PRO	4
1	A	63	ALA	4
1	A	120	ASP	4
1	A	100	ASN	3
1	A	29	SER	3
1	A	17	ASN	2
1	A	49	CYS	2
1	A	105	LEU	2
1	A	10	PRO	2
1	A	58	VAL	2
1	A	83	ASN	1
1	A	11	SER	1
1	A	62	GLU	1
1	A	76	SER	1
1	A	57	MET	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	96/103 (93%)	67±3 (70±3%)	29±3 (30±3%)	1 16
All	All	4800/5150 (93%)	3347 (70%)	1453 (30%)	1 16

All 76 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	105	LEU	50
1	A	93	SER	50

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Mol	Chain	Res	Type	Models (Total)
1	A	96	THR	50
1	A	119	SER	49
1	A	123	THR	49
1	A	31	ILE	48
1	A	71	CYS	47
1	A	32	THR	46
1	A	40	HIS	44
1	A	17	ASN	39
1	A	72	GLN	38
1	A	57	MET	37
1	A	51	LEU	34
1	A	19	GLN	34
1	A	67	GLU	34
1	A	44	GLU	31
1	A	47	SER	31
1	A	37	SER	30
1	A	13	ARG	29
1	A	14	ASP	28
1	A	66	CYS	27
1	A	62	GLU	27
1	A	50	GLU	27
1	A	21	ASP	26
1	A	81	ARG	26
1	A	120	ASP	26
1	A	70	LYS	25
1	A	104	SER	24
1	A	8	ARG	24
1	A	108	ASN	22
1	A	101	SER	22
1	A	60	ASN	22
1	A	46	LYS	22
1	A	34	SER	21
1	A	114	SER	20
1	A	26	ASP	17
1	A	11	SER	16
1	A	36	ASN	16
1	A	109	SER	16
1	A	79	ASN	16
1	A	29	SER	15
1	A	22	ILE	15
1	A	100	ASN	14
1	A	91	ASP	13

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Mol	Chain	Res	Type	Models (Total)
1	A	69	VAL	13
1	A	20	LEU	13
1	A	27	PHE	12
1	A	78	SER	12
1	A	45	SER	11
1	A	112	LEU	9
1	A	65	ILE	8
1	A	73	SER	8
1	A	58	VAL	8
1	A	16	ASP	7
1	A	83	ASN	6
1	A	30	SER	5
1	A	76	SER	5
1	A	42	ILE	4
1	A	98	SER	4
1	A	117	GLU	3
1	A	41	LEU	3
1	A	74	PRO	3
1	A	61	PRO	3
1	A	25	VAL	3
1	A	64	PRO	2
1	A	48	TYR	2
1	A	103	TYR	2
1	A	68	SER	2
1	A	35	CYS	1
1	A	90	THR	1
1	A	95	VAL	1
1	A	75	PRO	1
1	A	15	ILE	1
1	A	77	ILE	1
1	A	9	CYS	1
1	A	82	HIS	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

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided