



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 05:52 PM UTC

PDB ID : 1E5G / pdb_00001e5g
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

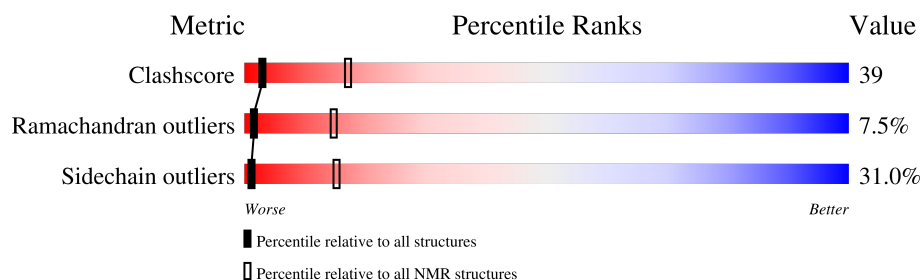
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	120	24% 58% 9% 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)	0.46	13
2	A:69-A:83, A:88-A:126 (54)	0.40	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 6 clusters and 3 single-model clusters were found.

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

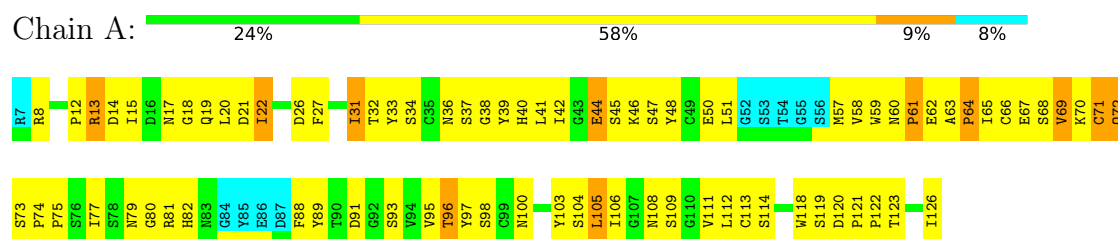
Mol	Chain	Residues	Atoms						Trace
1	A	120	Total	C	H	N	O	S	0
			1698	544	807	150	188	9	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3

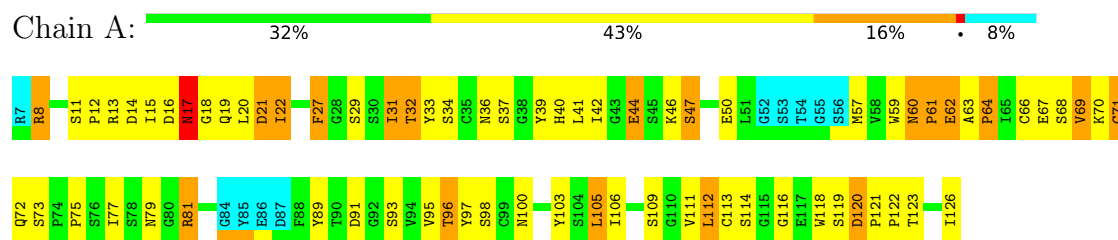


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

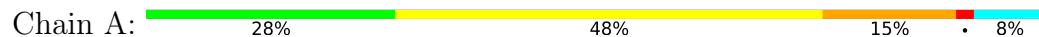
4.2.1 Score per residue for model 1

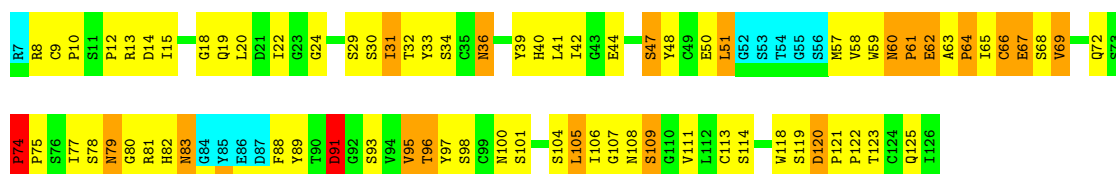
- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



4.2.2 Score per residue for model 2

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3

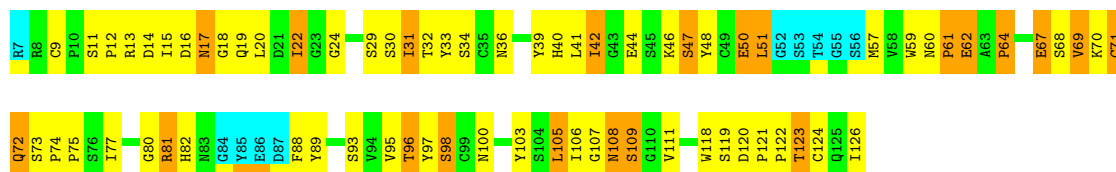




4.2.3 Score per residue for model 3

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3

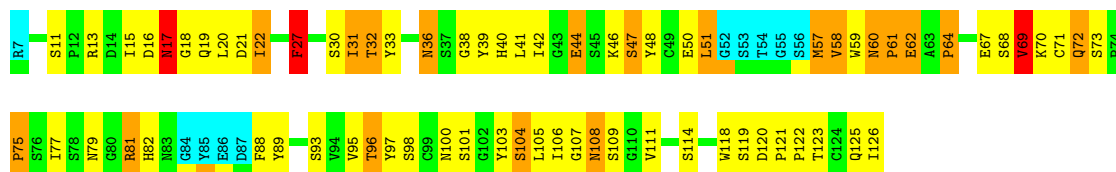
Chain A: 32% 42% 18% 8%



4.2.4 Score per residue for model 4

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3

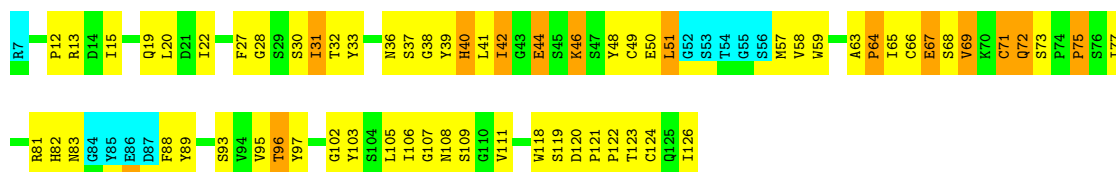
Chain A: 32% 42% 16% 8%



4.2.5 Score per residue for model 5

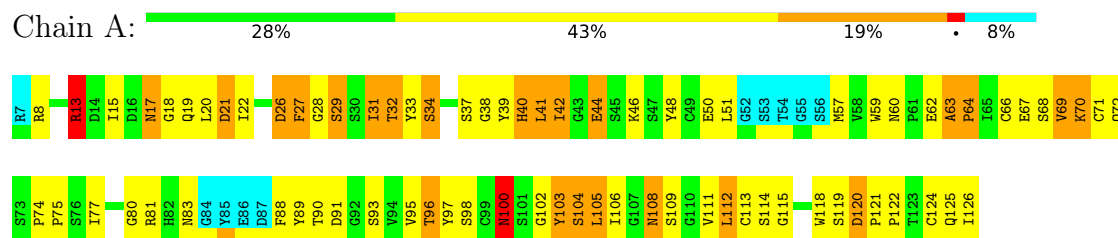
- Molecule 1: COMPLEMENT CONTROL PROTEIN C3

Chain A: 38% 43% 11% 8%



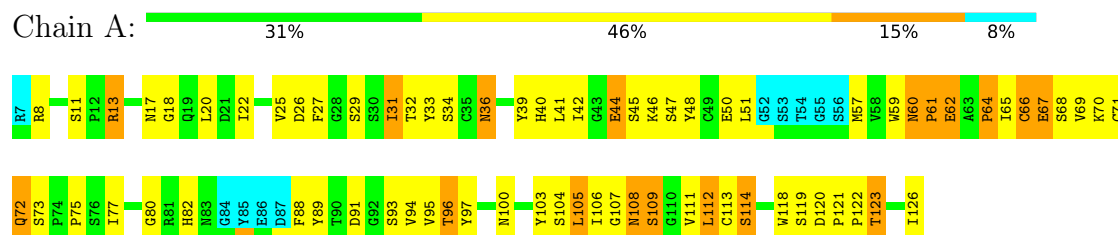
4.2.6 Score per residue for model 6

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



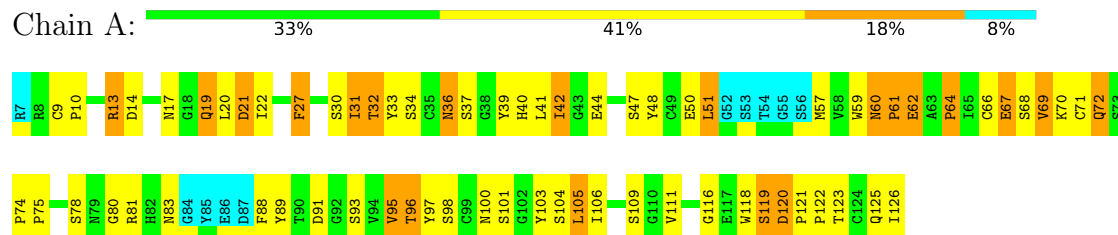
4.2.7 Score per residue for model 7

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



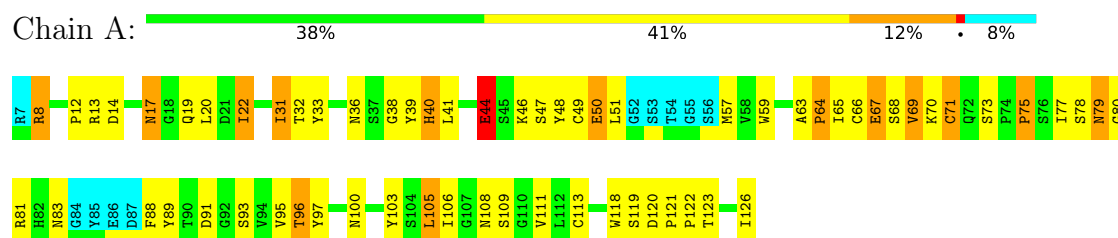
4.2.8 Score per residue for model 8

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



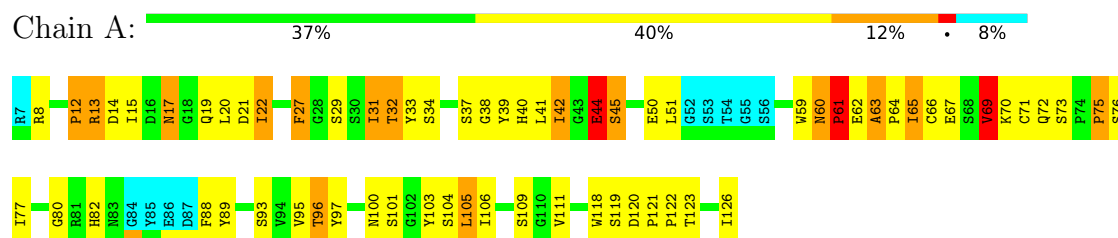
4.2.9 Score per residue for model 9

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



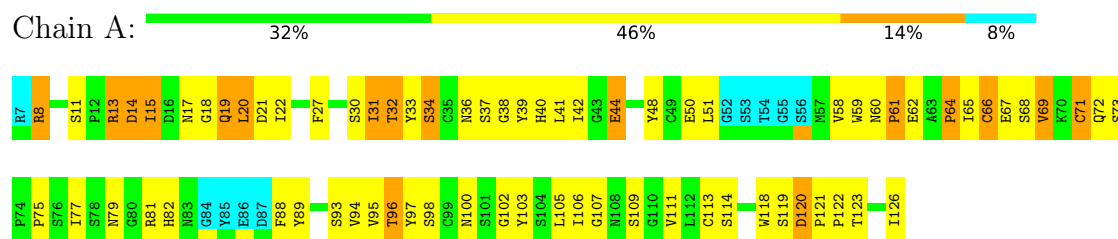
4.2.10 Score per residue for model 10

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



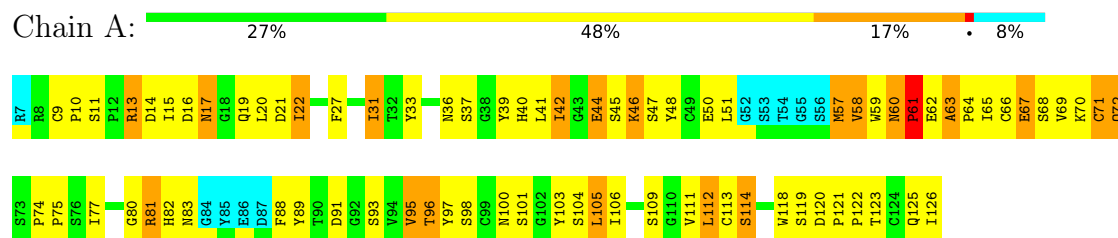
4.2.11 Score per residue for model 11

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



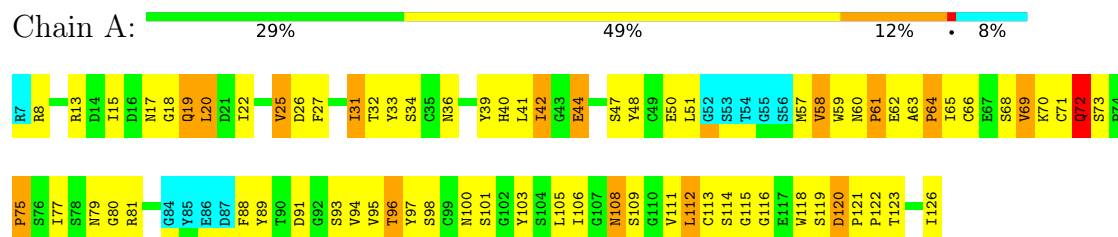
4.2.12 Score per residue for model 12

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



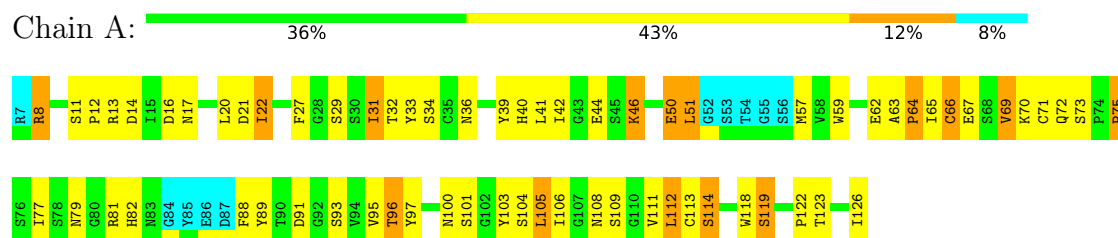
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



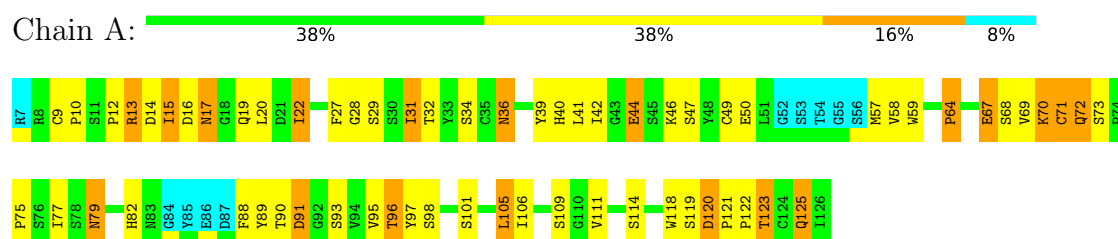
4.2.14 Score per residue for model 14

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



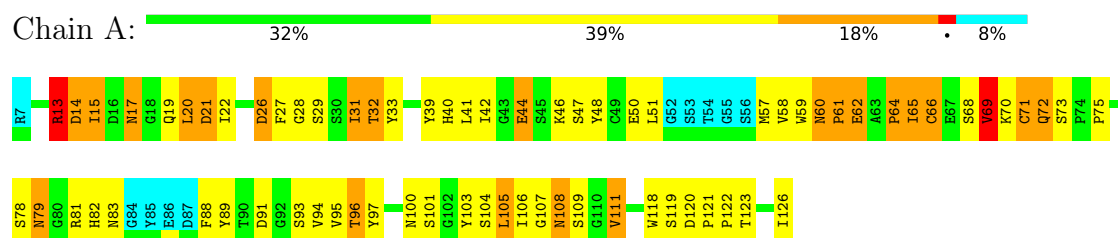
4.2.15 Score per residue for model 15

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



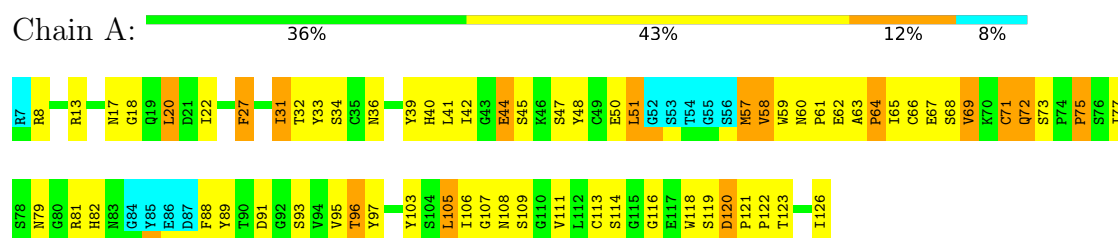
4.2.16 Score per residue for model 16

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



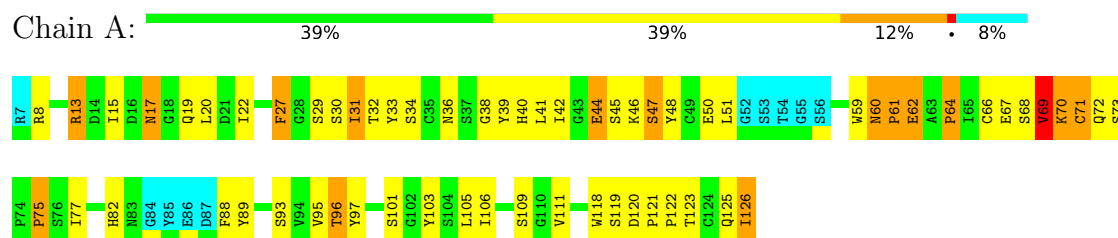
4.2.17 Score per residue for model 17

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



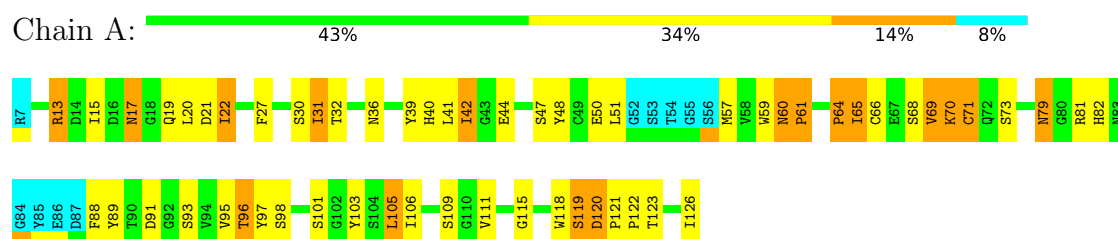
4.2.18 Score per residue for model 18

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



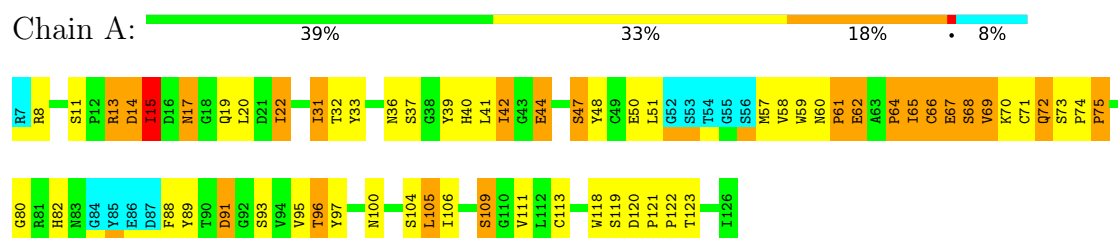
4.2.19 Score per residue for model 19

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



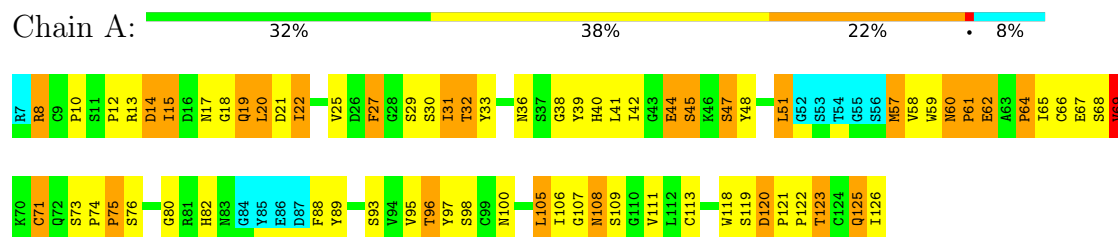
4.2.20 Score per residue for model 20

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



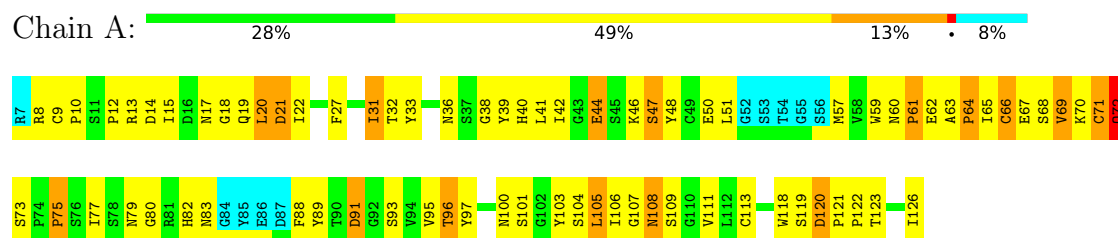
4.2.21 Score per residue for model 21

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



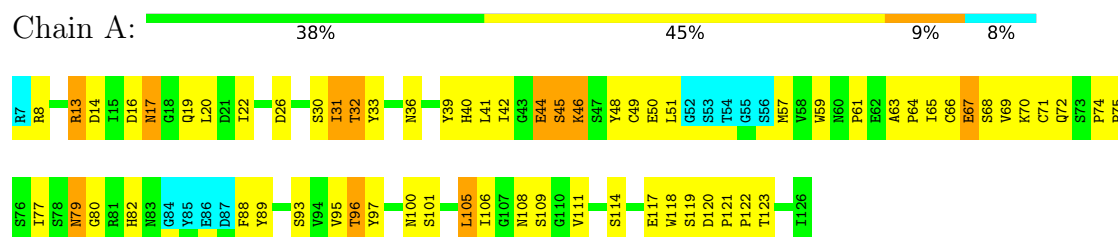
4.2.22 Score per residue for model 22

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



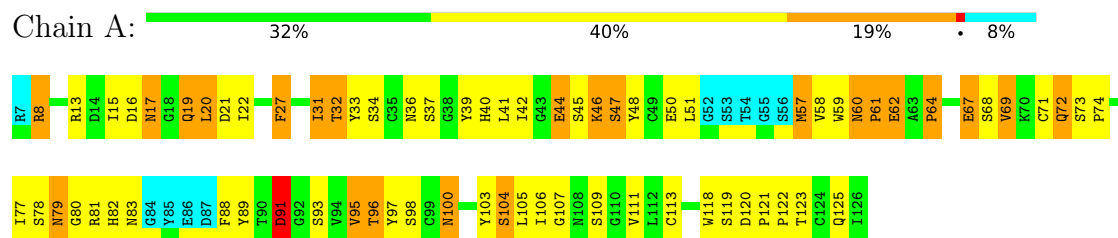
4.2.23 Score per residue for model 23

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



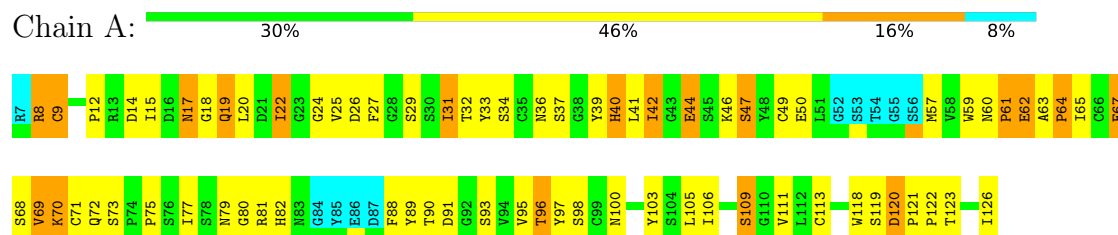
4.2.24 Score per residue for model 24

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



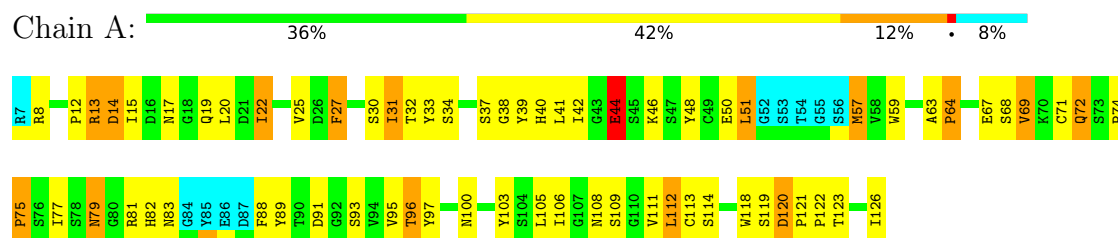
4.2.25 Score per residue for model 25

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



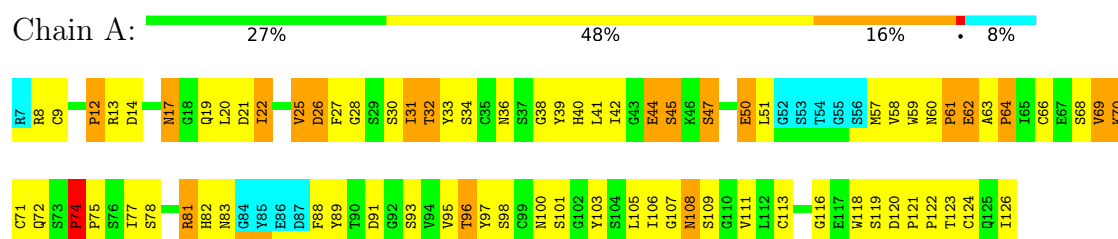
4.2.26 Score per residue for model 26

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



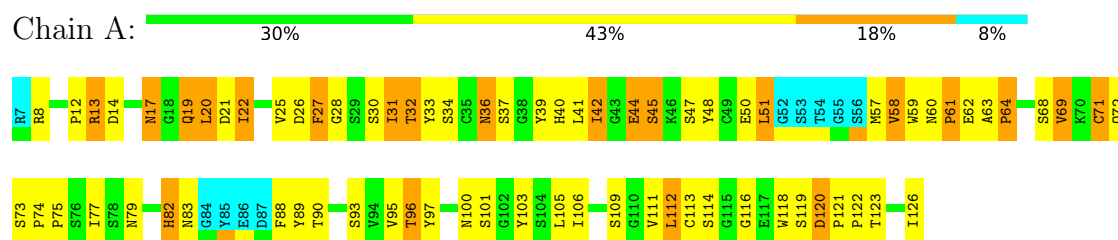
4.2.27 Score per residue for model 27

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



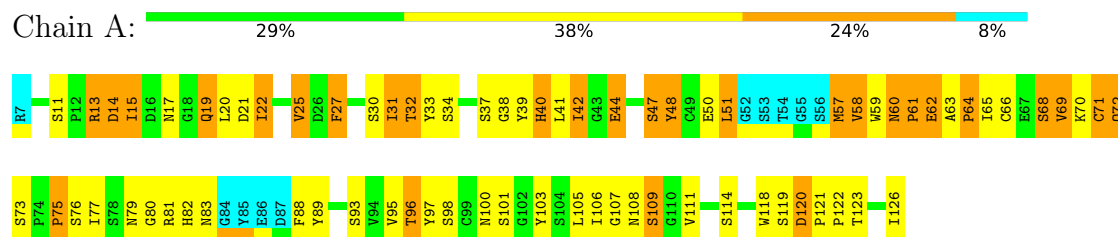
4.2.28 Score per residue for model 28

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



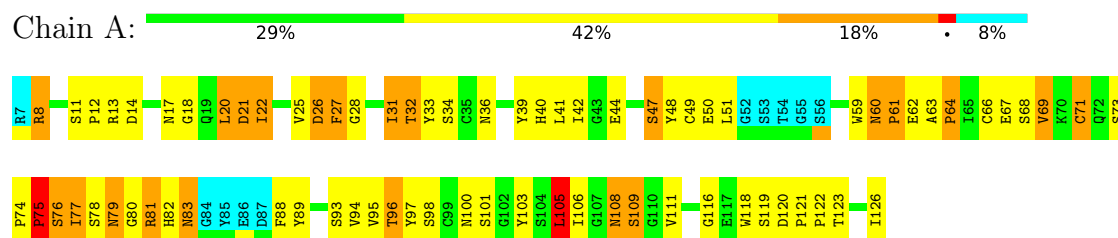
4.2.29 Score per residue for model 29

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



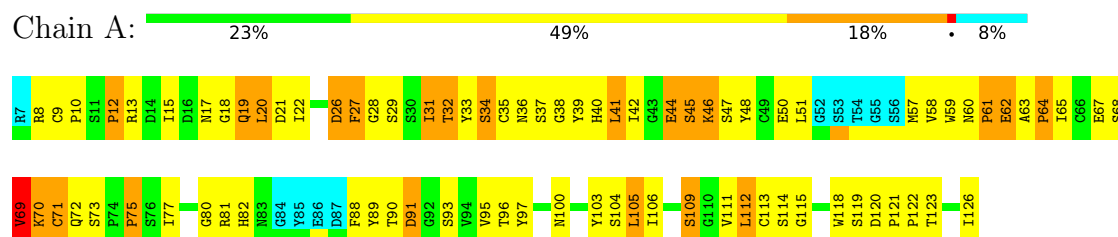
4.2.30 Score per residue for model 30

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



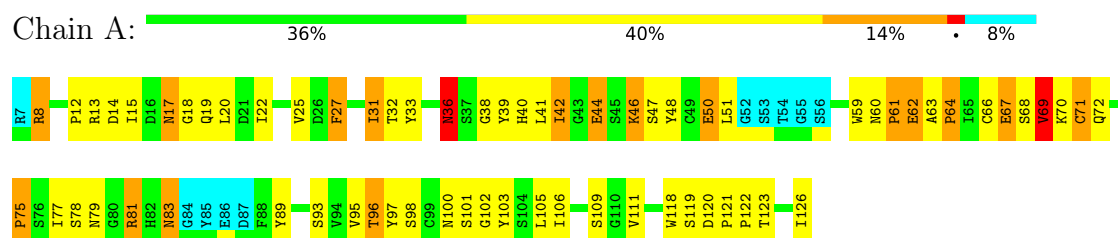
4.2.31 Score per residue for model 31

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



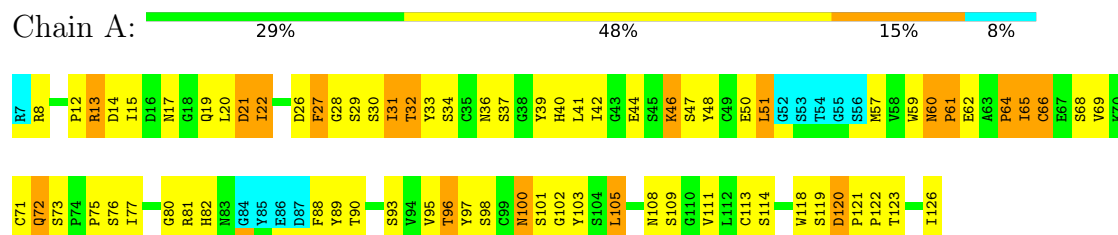
4.2.32 Score per residue for model 32

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



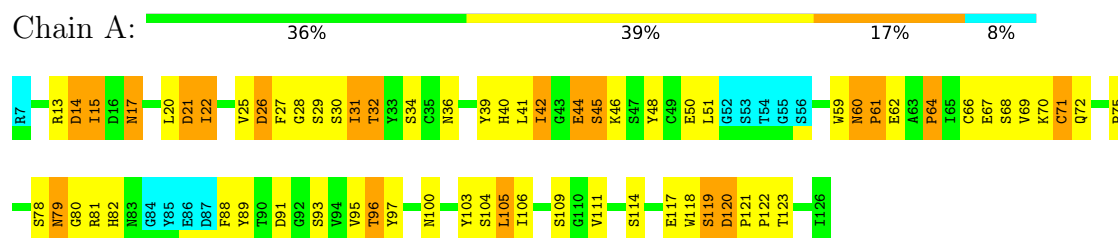
4.2.33 Score per residue for model 33

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



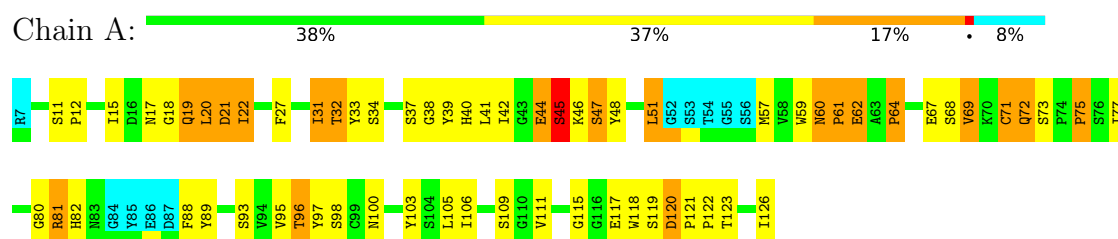
4.2.34 Score per residue for model 34

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



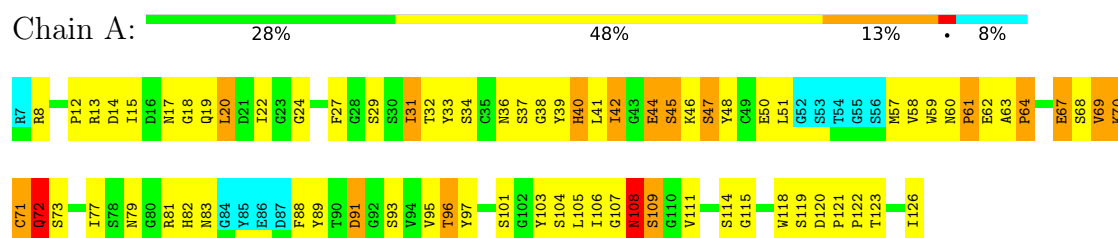
4.2.35 Score per residue for model 35

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



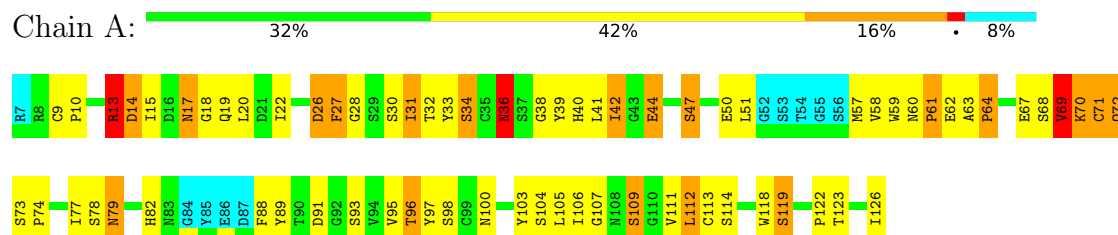
4.2.36 Score per residue for model 36

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



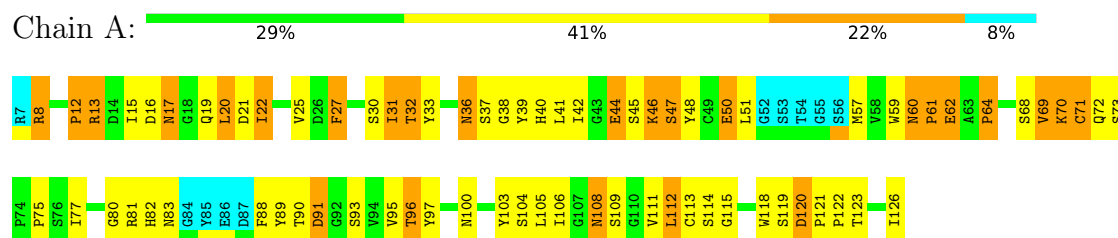
4.2.37 Score per residue for model 37

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



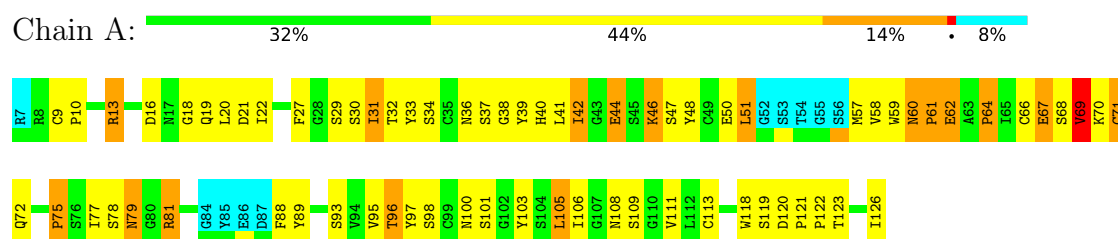
4.2.38 Score per residue for model 38

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



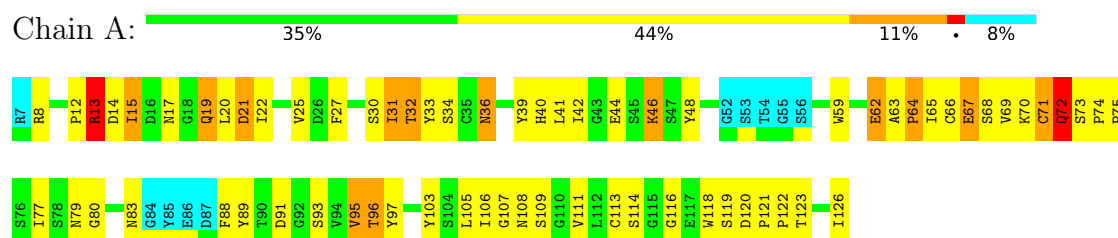
4.2.39 Score per residue for model 39

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



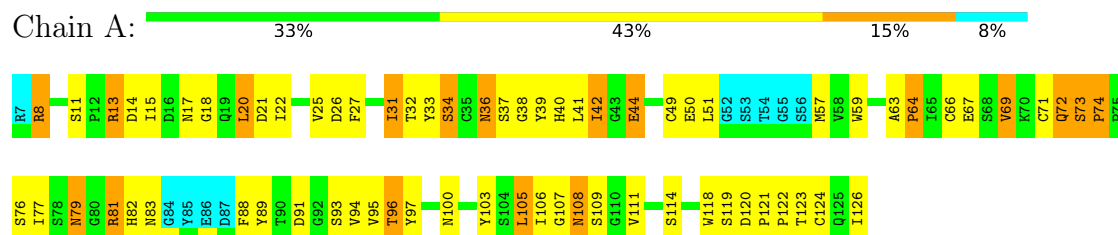
4.2.40 Score per residue for model 40

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



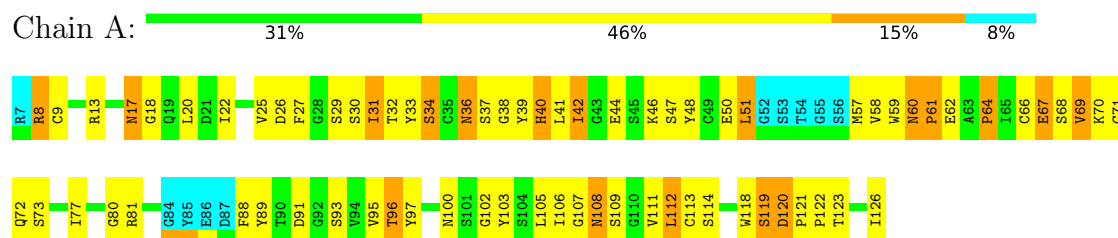
4.2.41 Score per residue for model 41

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



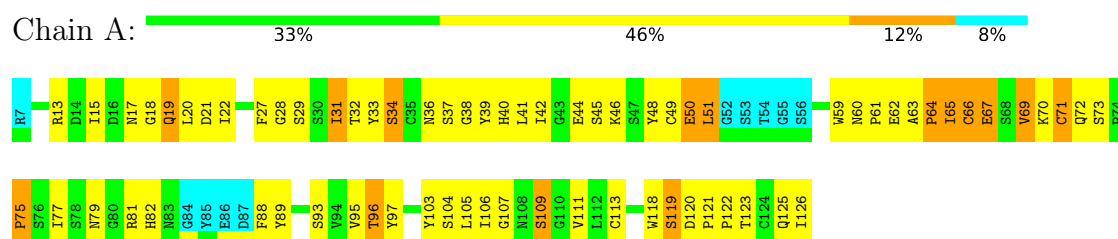
4.2.42 Score per residue for model 42

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



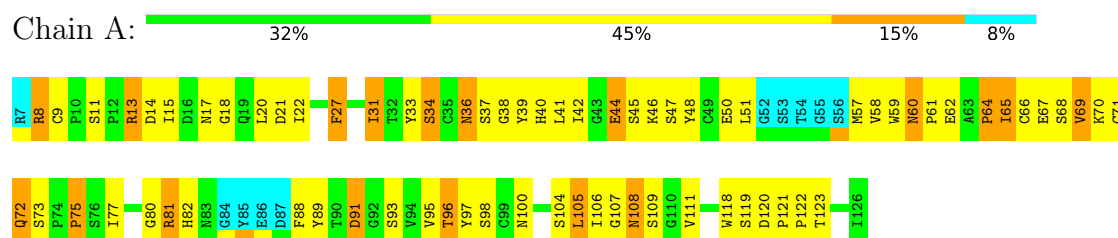
4.2.43 Score per residue for model 43

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



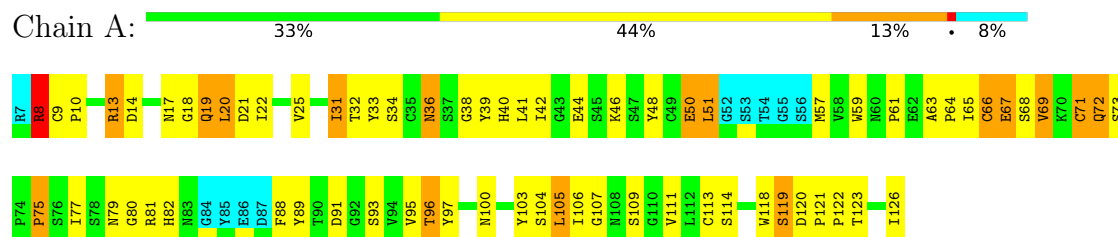
4.2.44 Score per residue for model 44

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



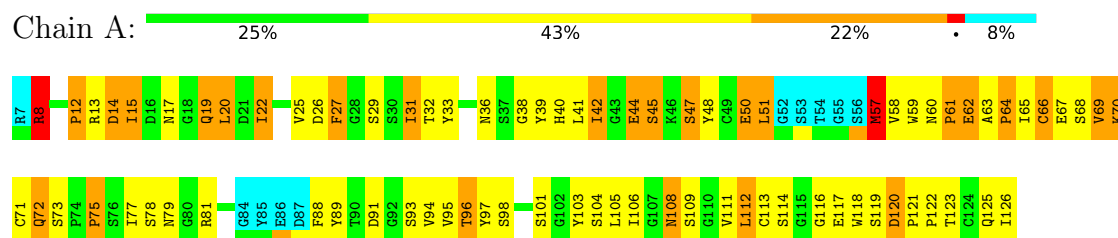
4.2.45 Score per residue for model 45

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



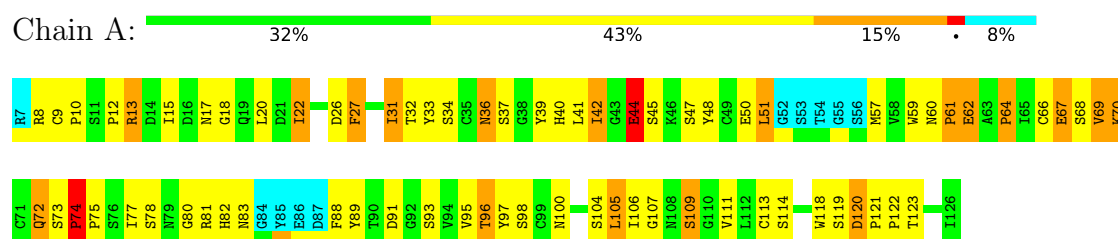
4.2.46 Score per residue for model 46

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



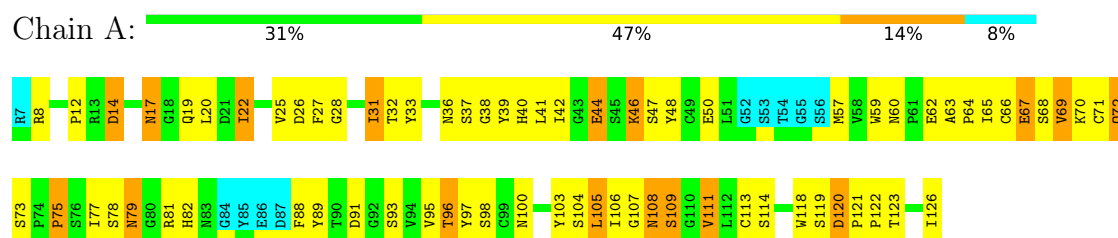
4.2.47 Score per residue for model 47

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



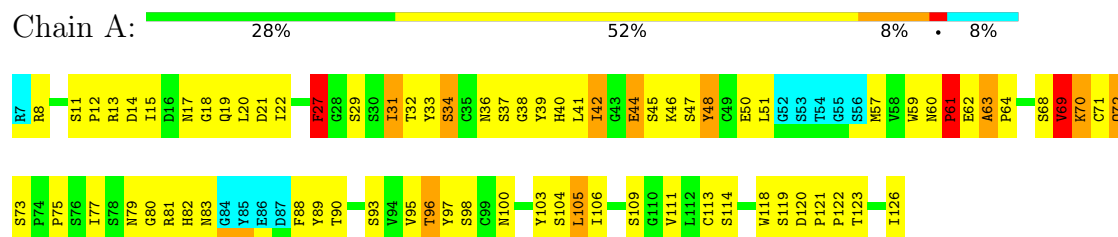
4.2.48 Score per residue for model 48

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



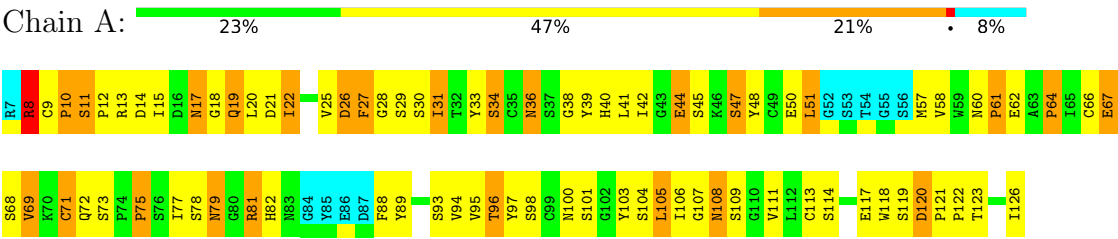
4.2.49 Score per residue for model 49

- Molecule 1: COMPLEMENT CONTROL PROTEIN C3



4.2.50 Score per residue for model 50

● Molecule 1: COMPLEMENT CONTROL PROTEIN C3



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.

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.34±0.04	0±0/841 (0.0± 0.0%)	0.67±0.04	0±0/1145 (0.0± 0.0%)
All	All	0.34	3/42050 (0.0%)	0.68	4/57250 (0.0%)

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

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	74	PRO	CA-C	-5.42	1.47	1.52	47	3

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	74	PRO	CB-CA-C	-6.59	102.88	110.92	27	3
1	A	75	PRO	N-CA-CB	-5.17	97.82	103.25	30	1

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	62±10
All	All	41000	37450	37352	3082

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 39.

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
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:19:GLN:C	1:A:20:LEU:HD13	0.83	1.99	21	2
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:41:LEU:C	1:A:42:ILE:HD13	0.79	2.02	6	13
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LEU:HD21	1:A:33:TYR:CZ	0.74	2.17	29	4
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:HD12	1:A:126:ILE:N	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:N	1:A:20:LEU:HD23	0.69	2.02	11	11
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
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:HD21	1:A:33:TYR:OH	0.69	1.87	2	4
1:A:20:LEU:HD22	1:A:33:TYR:CD2	0.69	2.22	11	6
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:C	1:A:20:LEU:HD11	0.68	2.14	21	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	4
1:A:41:LEU:HD23	1:A:41:LEU:O	0.66	1.91	29	3
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: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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:GLN:C	1:A:20:LEU:HD22	0.63	2.18	46	1
1:A:42:ILE:HD13	1:A:42:ILE:N	0.63	2.08	6	9
1:A:77:ILE:HD11	1:A:80:GLY:HA3	0.63	1.69	47	4
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:112:LEU:HD13	1:A:112:LEU:C	0.61	2.20	37	12
1:A:126:ILE:HG22	1:A:126:ILE:O	0.61	1.95	33	24
1:A:51:LEU:HD12	1:A:51:LEU:C	0.61	2.21	35	5
1:A:33:TYR:O	1:A:41:LEU:HD13	0.61	1.96	26	2
1:A:69:VAL:O	1:A:69:VAL:HG23	0.61	1.96	13	16
1:A:22:ILE:HD13	1:A:31:ILE:HD13	0.61	1.71	25	1
1:A:41:LEU:C	1:A:41:LEU:HD23	0.60	2.21	1	27
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
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: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:27:PHE:CE1	1:A:57:MET:HE1	0.59	2.31	4	1
1:A:25:VAL:HG22	1:A:59:TRP:HZ2	0.59	1.57	27	2
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	10
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:40:HIS:HB3	1:A:69:VAL:HG12	0.58	1.76	35	4
1:A:8:ARG:HD3	1:A:25:VAL:HG23	0.58	1.74	21	5
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LEU:HD13	1:A:20:LEU:N	0.57	2.14	35	2
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:75:PRO:CB	1:A:97:TYR:CE2	0.56	2.88	2	1
1:A:20:LEU:HD22	1:A:20:LEU:H	0.56	1.60	21	2
1:A:14:ASP:HA	1:A:20:LEU:HD11	0.56	1.77	25	5
1:A:15:ILE:HG22	1:A:20:LEU:HD21	0.56	1.76	10	3
1:A:111:VAL:HG13	1:A:119:SER:O	0.56	2.01	23	6
1:A:105:LEU:HD22	1:A:109:SER:HB2	0.56	1.77	33	4
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
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: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: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:20:LEU:CD2	1:A:33:TYR:CZ	0.54	2.91	29	3
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:97:TYR:CD1	1:A:111:VAL:HG21	0.54	2.37	3	10
1:A:14:ASP:C	1:A:20:LEU:HD21	0.54	2.27	46	3
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: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:39:TYR:CE2	1:A:68:SER:CB	0.53	2.92	20	3
1:A:105:LEU:HD22	1:A:109:SER:HB3	0.53	1.78	20	2
1:A:20:LEU:CD1	1:A:33:TYR:CE2	0.53	2.92	46	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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: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:40:HIS:CE1	1:A:42:ILE:CD1	0.52	2.92	14	33
1:A:77:ILE:HG23	1:A:97:TYR:HE2	0.52	1.65	23	16
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:N	1:A:126:ILE:CD1	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:88:PHE:C	1:A:89:TYR:CD2	0.52	2.88	19	24
1:A:9:CYS:SG	1:A:49:CYS:CB	0.52	2.98	25	1
1:A:88:PHE:C	1:A:89:TYR:CD1	0.51	2.89	27	24
1:A:25:VAL:HG12	1:A:59:TRP:CZ2	0.51	2.40	48	2
1:A:20:LEU:CG	1:A:33:TYR:CE1	0.51	2.92	40	2
1:A:33:TYR:CD1	1:A:62:GLU:O	0.51	2.64	22	20
1:A:74:PRO:HG3	1:A:118:TRP:CZ2	0.51	2.40	47	2
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:109:SER:O	1:A:111:VAL:HG23	0.51	2.05	27	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:63:ALA:HB1	1:A:64:PRO:C	0.50	2.31	10	3
1:A:48:TYR:CD1	1:A:60:ASN:CB	0.50	2.95	30	3
1:A:41:LEU:HD23	1:A:41:LEU:C	0.50	2.31	29	2
1:A:33:TYR:CG	1:A:63:ALA:O	0.50	2.64	6	2
1:A:96:THR:HG22	1:A:109:SER:HG	0.50	1.67	41	4
1:A:27:PHE:CD1	1:A:57:MET:HE1	0.50	2.41	4	1
1:A:112:LEU:HD22	1:A:112:LEU:C	0.50	2.32	31	4
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:112:LEU:C	1:A:112:LEU:HD13	0.50	2.32	31	1
1:A:106:ILE:HG22	1:A:107:GLY:N	0.50	2.22	27	22
1:A:33:TYR:CE2	1:A:63:ALA:C	0.50	2.90	6	1
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:33:TYR:CD2	1:A:63:ALA:C	0.49	2.90	6	2
1:A:69:VAL:HG12	1:A:69:VAL:O	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:HG13	1:A:69:VAL:O	0.49	2.08	40	3
1:A:33:TYR:CE1	1:A:62:GLU:C	0.49	2.91	36	6
1:A:70:LYS:HG2	1:A:88:PHE:CD1	0.49	2.43	46	1
1:A:15:ILE:HG23	1:A:18:GLY:C	0.49	2.32	50	14
1:A:51:LEU:HD12	1:A:51:LEU:O	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:77:ILE:HG23	1:A:97:TYR:CE2	0.48	2.43	45	10
1:A:20:LEU:N	1:A:20:LEU:CD2	0.48	2.74	16	6
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:60:ASN:O	1:A:61:PRO:C	0.48	2.57	10	36
1:A:83:ASN:OD1	1:A:95:VAL:HG12	0.48	2.08	2	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:51:LEU:C	1:A:58:VAL:HG22	0.48	2.34	11	5
1:A:12:PRO:CB	1:A:31:ILE:CD1	0.48	2.92	25	4
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:69:VAL:HG22	1:A:91:ASP:HB3	0.48	1.84	2	1
1:A:111:VAL:HG22	1:A:122:PRO:HD3	0.48	1.84	27	3
1:A:74:PRO:O	1:A:82:HIS:CE1	0.48	2.67	26	7
1:A:33:TYR:CE2	1:A:62:GLU:C	0.48	2.92	35	6
1:A:14:ASP:O	1:A:15:ILE:CG2	0.48	2.62	46	6
1:A:106:ILE:O	1:A:122:PRO:CB	0.48	2.62	7	49
1:A:40:HIS:CD2	1:A:40:HIS:O	0.48	2.67	19	10
1:A:74:PRO:CG	1:A:118:TRP:CZ2	0.48	2.96	47	2
1:A:39:TYR:CD1	1:A:67:GLU:O	0.48	2.66	36	2
1:A:123:THR:HG22	1:A:125:GLN:HE22	0.48	1.67	21	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: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:39:TYR:CD2	1:A:67:GLU:C	0.47	2.92	15	11
1:A:63:ALA:HB3	1:A:64:PRO:C	0.47	2.34	6	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:SER:C	1:A:48:TYR:CD2	0.47	2.92	44	2
1:A:11:SER:HG	1:A:12:PRO:C	0.47	2.18	50	1
1:A:20:LEU:N	1:A:20:LEU:CD1	0.47	2.77	15	2
1:A:74:PRO:O	1:A:82:HIS:CD2	0.47	2.67	30	3
1:A:120:ASP:HB3	1:A:121:PRO:C	0.47	2.34	42	1
1:A:31:ILE:HD12	1:A:47:SER:HB2	0.47	1.86	49	1
1:A:79:ASN:N	1:A:79:ASN:ND2	0.47	2.63	23	11
1:A:48:TYR:CD1	1:A:60:ASN:O	0.47	2.67	44	3
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: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:O	1:A:40:HIS:CG	0.47	2.67	31	18
1:A:105:LEU:HD22	1:A:109:SER:CB	0.47	2.39	20	3
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	8
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:14:ASP:C	1:A:15:ILE:CG1	0.47	2.88	20	1
1:A:100:ASN:CG	1:A:101:SER:N	0.46	2.73	4	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:72:GLN:CG	1:A:73:SER:N	0.46	2.77	36	7
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:11:SER:CB	1:A:12:PRO:C	0.46	2.89	50	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:41:LEU:CD2	1:A:44:GLU:O	0.46	2.64	12	4
1:A:17:ASN:ND2	1:A:17:ASN:N	0.46	2.63	16	12
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	36	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:44:GLU:C	1:A:64:PRO:CG	0.46	2.89	12	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: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:62:GLU:O	1:A:64:PRO:HD2	0.45	2.11	31	5
1:A:15:ILE:HG12	1:A:33:TYR:CE2	0.45	2.46	20	1
1:A:103:TYR:CD2	1:A:126:ILE:CD1	0.45	2.99	1	2
1:A:62:GLU:O	1:A:64:PRO:CD	0.45	2.64	29	7
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
1:A:39:TYR:CE2	1:A:68:SER:OG	0.45	2.69	20	1
1:A:25:VAL:O	1:A:25:VAL:CG1	0.45	2.64	29	2
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:77:ILE:CG2	1:A:122:PRO:O	0.45	2.65	27	6
1:A:15:ILE:HD11	1:A:66:CYS:HB2	0.45	1.87	6	1
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:89:TYR:CE2	1:A:95:VAL:CG1	0.45	3.00	6	1
1:A:70:LYS:HD2	1:A:88:PHE:CG	0.45	2.47	37	1
1:A:74:PRO:HB2	1:A:82:HIS:CG	0.45	2.47	27	3
1:A:17:ASN:HB3	1:A:39:TYR:CE2	0.45	2.47	18	7
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:CYS:N	1:A:89:TYR:O	0.45	2.50	38	8
1:A:10:PRO:HD2	1:A:59:TRP:CD1	0.45	2.47	2	10
1:A:33:TYR:CE1	1:A:63:ALA:O	0.45	2.70	6	1
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:125:GLN:C	1:A:126:ILE:HD12	0.45	2.37	18	1
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:44:GLU:O	1:A:64:PRO:CG	0.44	2.65	44	27
1:A:40:HIS:CD2	1:A:40:HIS:N	0.44	2.86	42	5
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:11:SER:HB3	1:A:12:PRO:C	0.44	2.37	50	1
1:A:65:ILE:HG22	1:A:66:CYS:H	0.44	1.72	43	7
1:A:50:GLU:O	1:A:58:VAL:N	0.44	2.50	13	1
1:A:63:ALA:O	1:A:64:PRO:O	0.44	2.36	31	5
1:A:31:ILE:CD1	1:A:47:SER:OG	0.44	2.66	50	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:111:VAL:CG1	1:A:118:TRP:HB3	0.44	2.42	27	3
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:18:GLY:CA	1:A:34:SER:O	0.44	2.66	47	19
1:A:15:ILE:CG2	1:A:18:GLY:C	0.44	2.91	35	15
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:17:ASN:N	1:A:17:ASN:ND2	0.44	2.65	3	2
1:A:33:TYR:CE2	1:A:62:GLU:CB	0.44	3.01	7	1
1:A:33:TYR:CD1	1:A:63:ALA:C	0.44	2.95	10	1
1:A:12:PRO:HG2	1:A:22:ILE:CD1	0.44	2.43	35	1
1:A:20:LEU:HD12	1:A:20:LEU:N	0.44	2.28	40	1
1:A:33:TYR:CZ	1:A:62:GLU:C	0.44	2.95	27	3
1:A:104:SER:CB	1:A:125:GLN:O	0.44	2.66	6	4
1:A:44:GLU:CD	1:A:61:PRO:CB	0.44	2.91	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:40:HIS:O	1:A:40:HIS:CD2	0.43	2.71	11	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: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:123:THR:HG22	1:A:125:GLN:NE2	0.43	2.28	21	1
1:A:44:GLU:O	1:A:64:PRO:CB	0.43	2.67	33	9
1:A:20:LEU:CG	1:A:33:TYR:CZ	0.43	3.02	2	1
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
1:A:97:TYR:CD2	1:A:111:VAL:CG2	0.43	3.01	34	3
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:70:LYS:CE	1:A:71:CYS:C	0.43	2.92	37	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:39:TYR:CD1	1:A:67:GLU:C	0.43	2.96	10	4
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:27:PHE:CZ	1:A:51:LEU:HG	0.43	2.48	31	4
1:A:88:PHE:O	1:A:89:TYR:CD2	0.43	2.71	19	1
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:73:SER:OG	1:A:82:HIS:NE2	0.43	2.52	29	17
1:A:97:TYR:CD1	1:A:111:VAL:CG2	0.43	3.02	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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: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:44:GLU:C	1:A:64:PRO:HG2	0.43	2.39	12	1
1:A:105:LEU:CD1	1:A:122:PRO:HB2	0.43	2.44	44	4
1:A:14:ASP:CG	1:A:15:ILE:N	0.43	2.77	22	1
1:A:76:SER:OG	1:A:77:ILE:N	0.43	2.52	30	1
1:A:24:GLY:O	1:A:29:SER:CB	0.42	2.67	2	3
1:A:105:LEU:HA	1:A:123:THR:O	0.42	2.14	3	2
1:A:83:ASN:ND2	1:A:96:THR:O	0.42	2.52	47	5
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:9:CYS:HB3	1:A:59:TRP:NE1	0.42	2.28	15	11
1:A:24:GLY:C	1:A:29:SER:CB	0.42	2.92	3	2
1:A:12:PRO:HB3	1:A:31:ILE:CD1	0.42	2.43	26	8
1:A:48:TYR:CD1	1:A:48:TYR:N	0.42	2.86	5	2
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:CD1	1:A:20:LEU:N	0.42	2.82	40	1
1:A:31:ILE:O	1:A:46:LYS:CG	0.42	2.68	4	8
1:A:105:LEU:CD1	1:A:109:SER:HA	0.42	2.45	7	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:69:VAL:HG21	1:A:115:GLY:H	0.42	1.75	13	1
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:38:GLY:CA	1:A:91:ASP:CG	0.42	2.93	31	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:91:ASP:OD1	1:A:115:GLY:N	0.42	2.53	38	2
1:A:72:GLN:O	1:A:118:TRP:NE1	0.42	2.48	37	2
1:A:113:CYS:HB2	1:A:118:TRP:CH2	0.42	2.50	43	9
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:70:LYS:HE3	1:A:71:CYS:C	0.42	2.40	37	1
1:A:112:LEU:C	1:A:112:LEU:CD1	0.42	2.91	38	2
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: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:39:TYR:C	1:A:69:VAL:HG13	0.42	2.40	48	1
1:A:107:GLY:O	1:A:108:ASN:CG	0.42	2.63	48	6
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:38:GLY:O	1:A:69:VAL:CG2	0.42	2.68	9	1
1:A:48:TYR:O	1:A:50:GLU:N	0.42	2.53	9	1
1:A:69:VAL:O	1:A:69:VAL:CG2	0.42	2.67	13	1
1:A:112:LEU:HD13	1:A:112:LEU:O	0.42	2.14	46	2
1:A:44:GLU:CD	1:A:61:PRO:CG	0.42	2.93	43	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:ILE:O	1:A:46:LYS:CE	0.41	2.68	40	1
1:A:16:ASP:C	1:A:18:GLY:N	0.41	2.78	1	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:47:SER:C	1:A:48:TYR:CD1	0.41	2.98	36	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: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: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:41:LEU:C	1:A:41:LEU:CD2	0.41	2.93	39	1
1:A:75:PRO:HA	1:A:97:TYR:CZ	0.41	2.51	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:81:ARG:CD	1:A:100:ASN:OD1	0.41	2.68	49	2
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: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
1:A:26:ASP:OD1	1:A:27:PHE:N	0.41	2.52	13	1
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:74:PRO:O	1:A:82:HIS:ND1	0.41	2.54	2	1
1:A:119:SER:O	1:A:120:ASP:CG	0.41	2.64	42	2
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: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:126:ILE:O	1:A:126:ILE:HG22	0.41	2.15	37	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: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:42:ILE:O	1:A:64:PRO:HB2	0.41	2.16	12	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:79:ASN:ND2	1:A:79:ASN:N	0.41	2.69	30	1
1:A:105:LEU:HD12	1:A:109:SER:CB	0.41	2.45	30	1
1:A:17:ASN:C	1:A:36:ASN:ND2	0.41	2.79	32	1
1:A:51:LEU:C	1:A:51:LEU:CD1	0.41	2.91	35	1
1:A:47:SER:OG	1:A:60:ASN:O	0.41	2.37	46	1
1:A:10:PRO:O	1:A:11:SER:C	0.41	2.64	50	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:49:CYS:HB2	1:A:59:TRP:CH2	0.40	2.51	41	1
1:A:103:TYR:CE1	1:A:126:ILE:HD11	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
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:75:PRO:HA	1:A:97:TYR:CE2	0.40	2.51	2	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:VAL:HG23	1:A:69:VAL:O	0.40	2.17	42	1
1:A:44:GLU:OE1	1:A:61:PRO:CG	0.40	2.69	43	1
1:A:42:ILE:N	1:A:42:ILE:HD13	0.40	2.32	48	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%)	1	15
All	All	5450/6000 (91%)	4020 (74%)	1020 (19%)	410 (8%)	1	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
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

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Mol	Chain	Res	Type	Models (Total)
1	A	100	ASN	3
1	A	29	SER	3
1	A	17	ASN	2
1	A	105	LEU	2
1	A	49	CYS	2
1	A	58	VAL	2
1	A	10	PRO	2
1	A	62	GLU	1
1	A	76	SER	1
1	A	83	ASN	1
1	A	57	MET	1
1	A	11	SER	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	96/103 (93%)	66±4 (69±4%)	30±4 (31±4%)	1	15
All	All	4800/5150 (93%)	3310 (69%)	1490 (31%)	1	15

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	31	ILE	50
1	A	93	SER	50
1	A	96	THR	50
1	A	105	LEU	50
1	A	119	SER	49
1	A	123	THR	49
1	A	71	CYS	48
1	A	17	ASN	47
1	A	32	THR	46
1	A	19	GLN	41
1	A	57	MET	40
1	A	44	GLU	37
1	A	72	GLN	37

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Mol	Chain	Res	Type	Models (Total)
1	A	67	GLU	36
1	A	50	GLU	35
1	A	70	LYS	32
1	A	46	LYS	28
1	A	47	SER	28
1	A	66	CYS	28
1	A	81	ARG	28
1	A	37	SER	26
1	A	62	GLU	26
1	A	13	ARG	26
1	A	22	ILE	25
1	A	51	LEU	25
1	A	8	ARG	24
1	A	14	ASP	24
1	A	42	ILE	24
1	A	108	ASN	23
1	A	104	SER	23
1	A	60	ASN	22
1	A	30	SER	22
1	A	21	ASP	21
1	A	101	SER	21
1	A	34	SER	20
1	A	120	ASP	20
1	A	114	SER	20
1	A	36	ASN	19
1	A	79	ASN	17
1	A	20	LEU	17
1	A	29	SER	15
1	A	109	SER	15
1	A	11	SER	14
1	A	100	ASN	14
1	A	112	LEU	13
1	A	78	SER	13
1	A	69	VAL	13
1	A	65	ILE	13
1	A	26	ASP	13
1	A	58	VAL	11
1	A	45	SER	11
1	A	91	ASP	8
1	A	16	ASP	8
1	A	73	SER	7
1	A	40	HIS	7

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Mol	Chain	Res	Type	Models (Total)
1	A	27	PHE	6
1	A	83	ASN	6
1	A	95	VAL	6
1	A	98	SER	5
1	A	76	SER	5
1	A	117	GLU	5
1	A	74	PRO	3
1	A	61	PRO	3
1	A	25	VAL	3
1	A	41	LEU	2
1	A	125	GLN	2
1	A	111	VAL	2
1	A	68	SER	2
1	A	48	TYR	2
1	A	103	TYR	1
1	A	126	ILE	1
1	A	15	ILE	1
1	A	9	CYS	1
1	A	82	HIS	1
1	A	90	THR	1
1	A	75	PRO	1
1	A	77	ILE	1
1	A	35	CYS	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 oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided