



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 09:55 AM UTC

PDB ID : 2M8L / pdb_00002m8l
BMRB ID : 19261
Title : HIV capsid dimer structure
Authors : Deshmukh, L.; Schwieters, C.D.; Grishaev, A.; Clore, G.; Ghirlando, R.
Deposited on : 2013-05-23

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
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

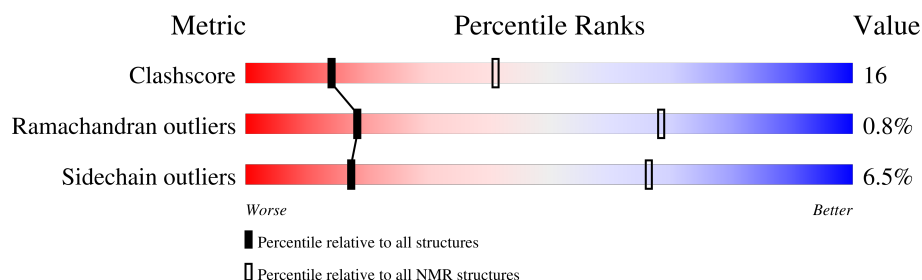
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR, SOLUTION SCATTERING

The overall completeness of chemical shifts assignment is 15%.

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	231	
1	B	231	

2 Ensemble composition and analysis

This entry contains 100 models. Model 95 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:1-A:145 (145)	0.05	95
2	A:150-A:221, B:150-B:221 (144)	0.06	1
3	B:1-B:145 (145)	0.06	38

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 11 clusters and 7 single-model clusters were found.

Cluster number	Models
1	1, 4, 5, 6, 9, 10, 11, 14, 15, 16, 19, 20, 25, 26, 29, 30, 32, 33, 36, 39, 40, 41, 44, 45, 48, 53, 54, 56, 61, 64, 65, 67, 68, 71, 77, 78, 81, 84, 87, 91, 94, 95
2	7, 12, 22, 27, 42, 47, 55, 57, 62, 66, 72, 80, 86, 96
3	3, 8, 18, 28, 38, 43, 51
4	24, 31, 49, 52, 59, 74, 76
5	34, 69, 79, 83, 89
6	2, 17, 37, 82
7	23, 58, 73, 98
8	21, 60, 75, 99
9	13, 63
10	70, 85
11	50, 97
Single-model clusters	35; 46; 88; 90; 92; 93; 100

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 6914 atoms, of which 3464 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Capsid protein p24.

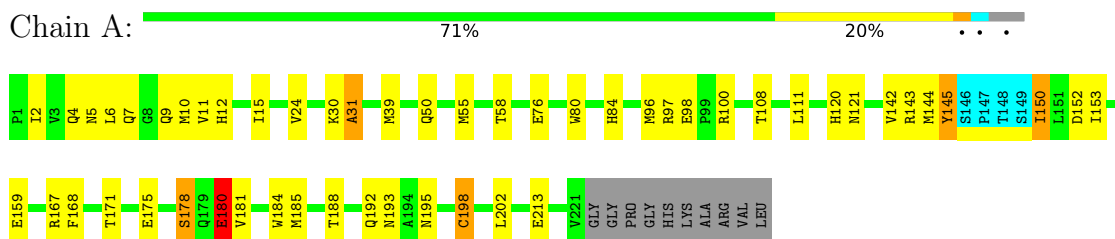
Mol	Chain	Residues	Atoms						Trace
1	A	221	Total	C	H	N	O	S	0
			3457	1088	1732	301	323	13	
1	B	221	Total	C	H	N	O	S	0
			3457	1088	1732	301	323	13	

4 Residue-property plots

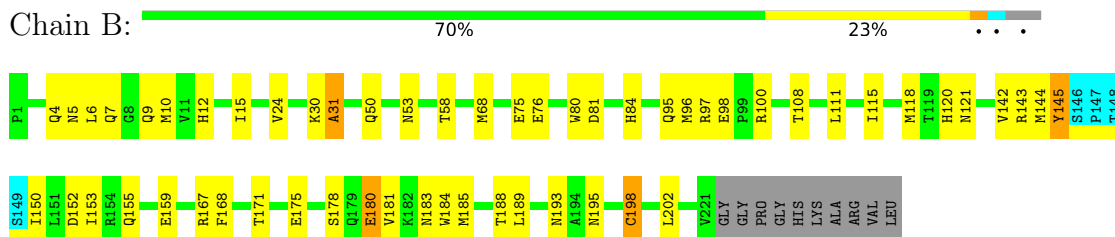
4.1 Average score per residue in the NMR ensemble

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: Capsid protein p24



- Molecule 1: Capsid protein p24

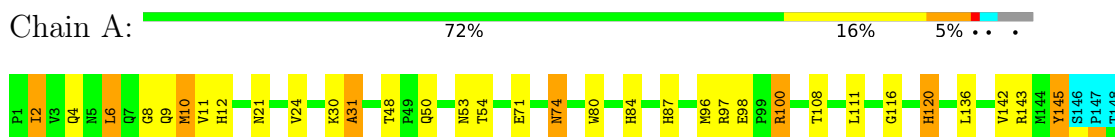


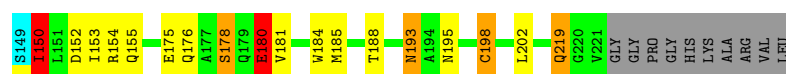
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

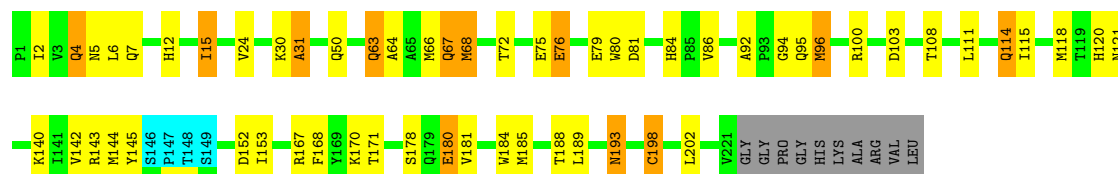
- Molecule 1: Capsid protein p24





• Molecule 1: Capsid protein p24

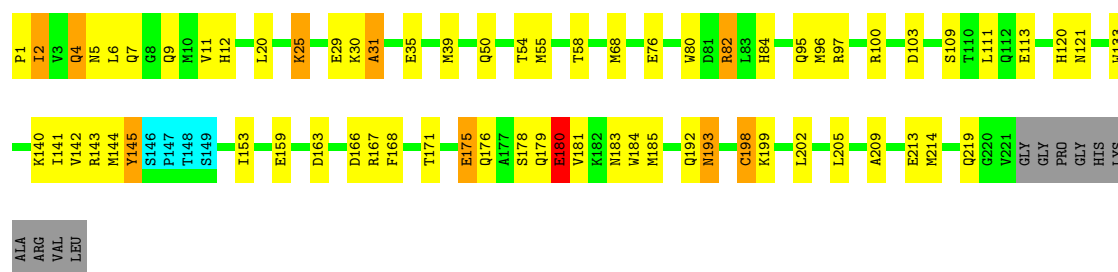
Chain B: 69% 20% 5% . . .



4.2.2 Score per residue for model 2

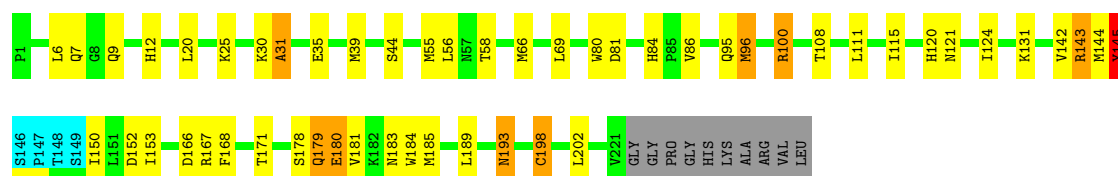
• Molecule 1: Capsid protein p24

Chain A: 65% 25% . . .



• Molecule 1: Capsid protein p24

Chain B: 71% 19% . . .



4.2.3 Score per residue for model 3

• Molecule 1: Capsid protein p24

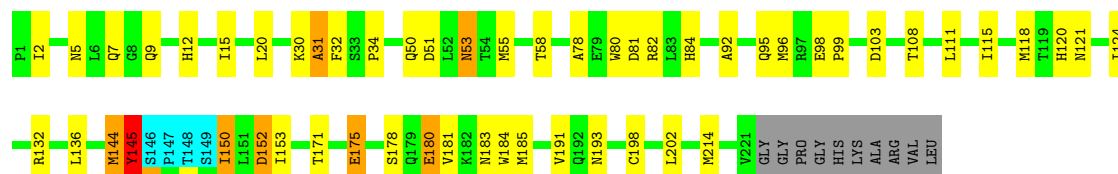
Chain A: 73% 16% . . .





• Molecule 1: Capsid protein p24

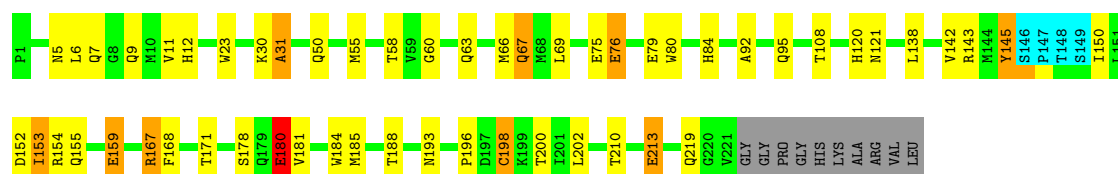
Chain B: 71% 20%



4.2.4 Score per residue for model 4

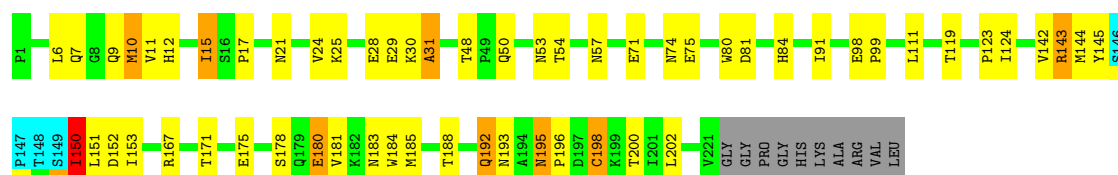
• Molecule 1: Capsid protein p24

Chain A: 71% 19%



• Molecule 1: Capsid protein p24

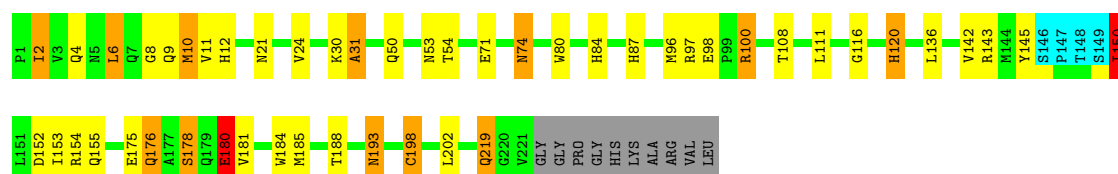
Chain B: 69% 21%



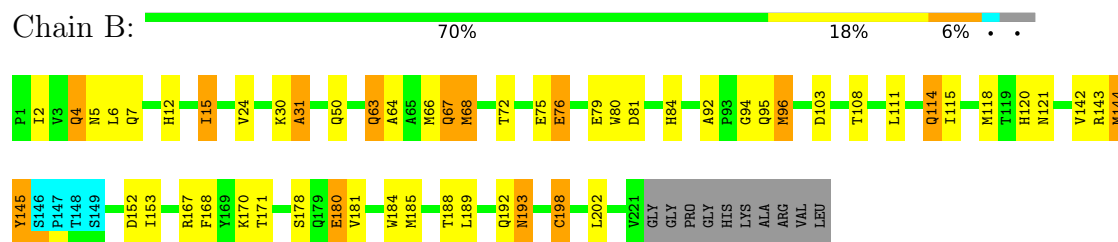
4.2.5 Score per residue for model 5

• Molecule 1: Capsid protein p24

Chain A: 73% 15% 5%

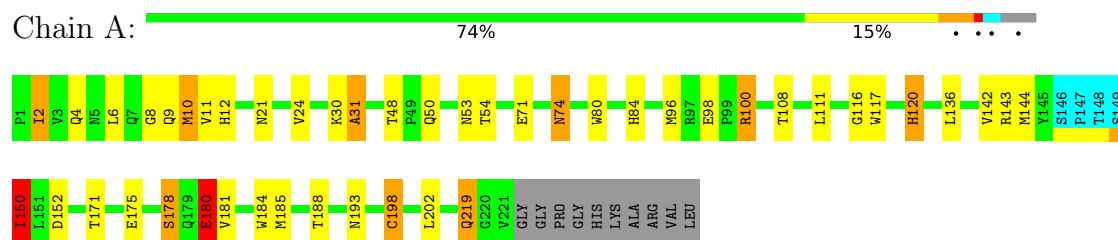


• Molecule 1: Capsid protein p24

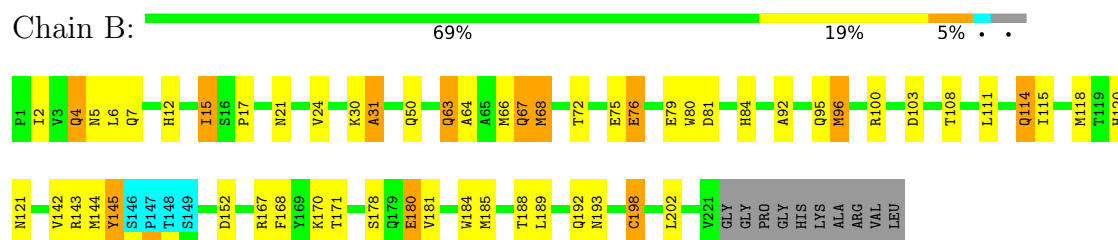


4.2.6 Score per residue for model 6

- Molecule 1: Capsid protein p24

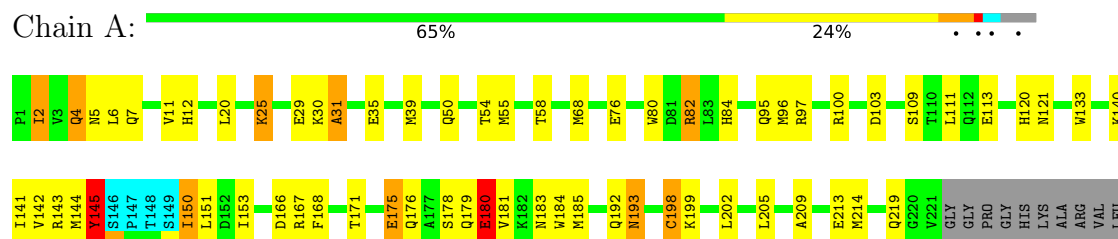


- Molecule 1: Capsid protein p24

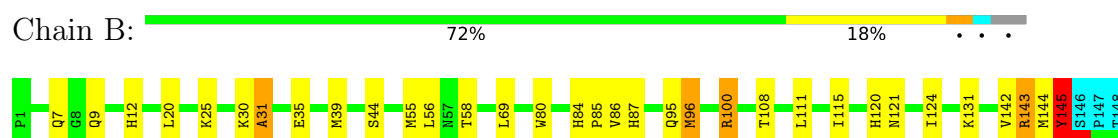


4.2.7 Score per residue for model 7

- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24



4.2.8 Score per residue for model 8

- Molecule 1: Capsid protein p24

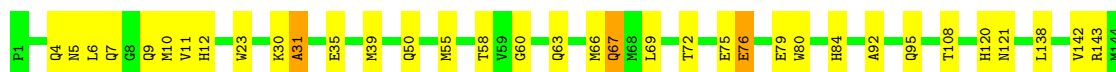


- Molecule 1: Capsid protein p24



4.2.9 Score per residue for model 9

- Molecule 1: Capsid protein p24

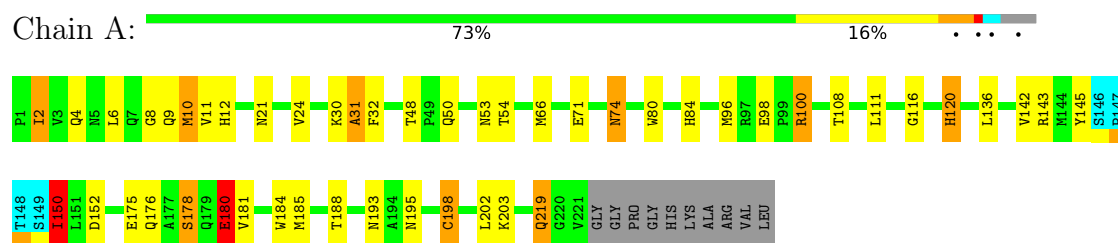


- Molecule 1: Capsid protein p24

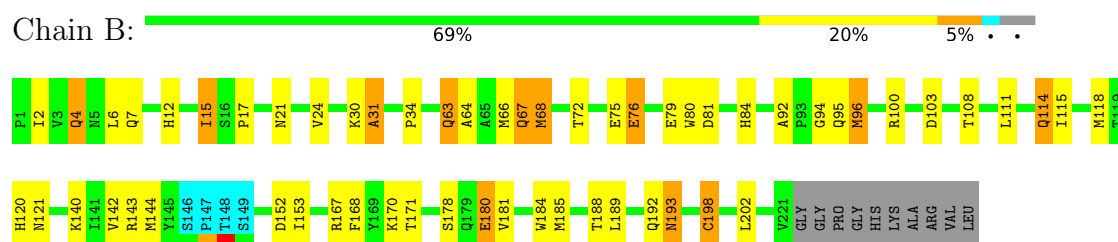


4.2.10 Score per residue for model 10

- Molecule 1: Capsid protein p24

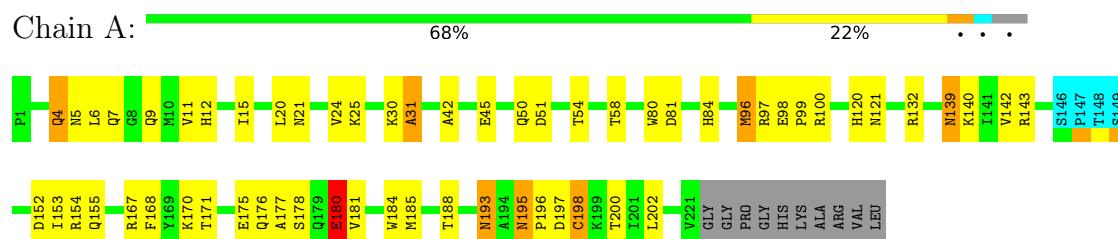


- Molecule 1: Capsid protein p24

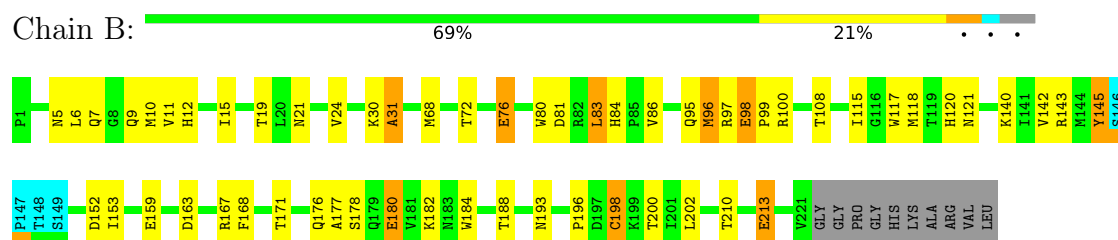


4.2.11 Score per residue for model 11

- Molecule 1: Capsid protein p24

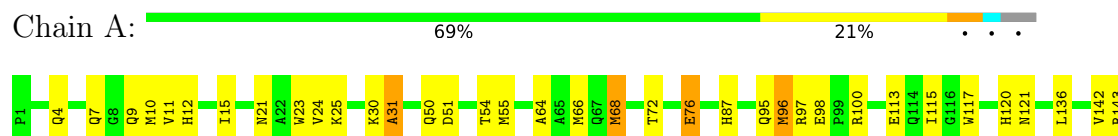


- Molecule 1: Capsid protein p24

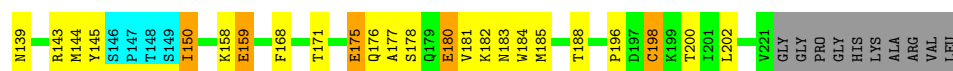
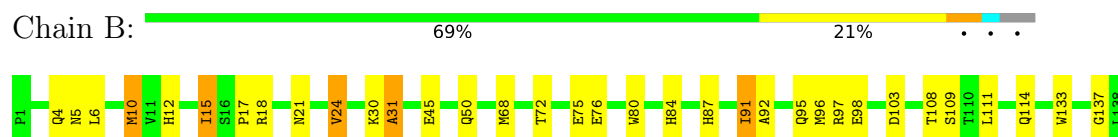


4.2.12 Score per residue for model 12

- Molecule 1: Capsid protein p24

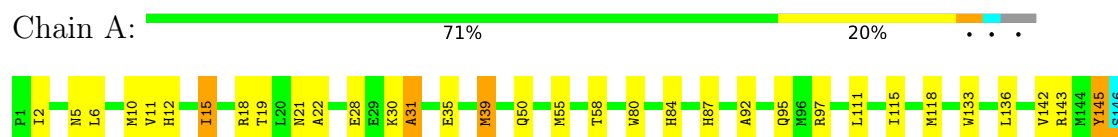


- Molecule 1: Capsid protein p24

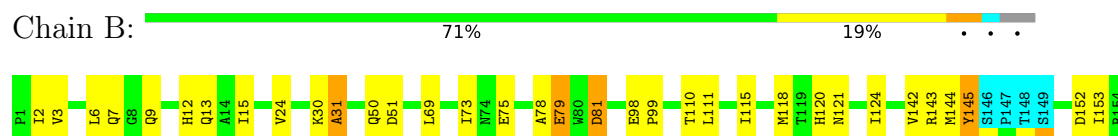


4.2.13 Score per residue for model 13

- Molecule 1: Capsid protein p24

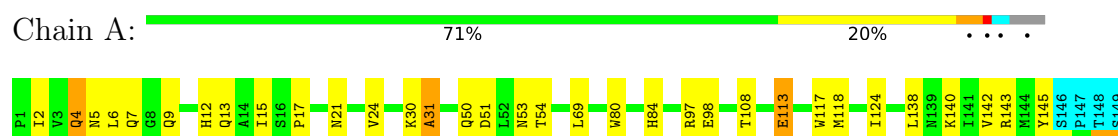


- Molecule 1: Capsid protein p24



4.2.14 Score per residue for model 14

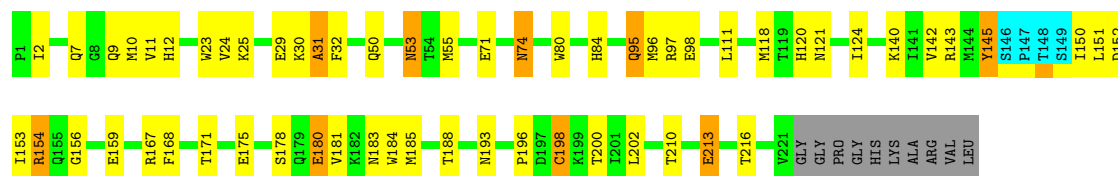
- Molecule 1: Capsid protein p24





• Molecule 1: Capsid protein p24

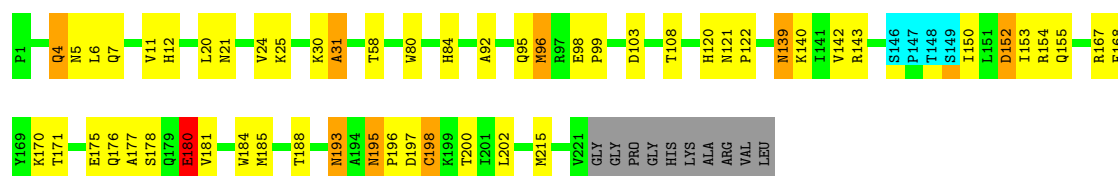
Chain B: 68% 22%



4.2.15 Score per residue for model 15

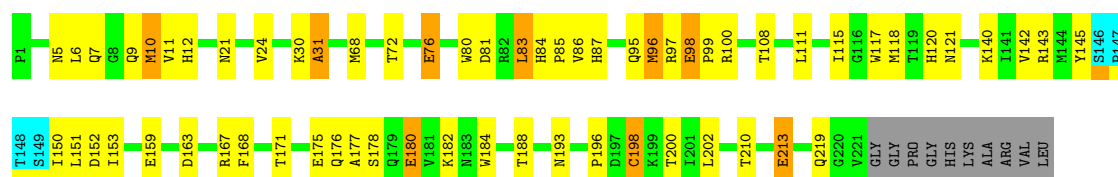
• Molecule 1: Capsid protein p24

Chain A: 70% 20%



• Molecule 1: Capsid protein p24

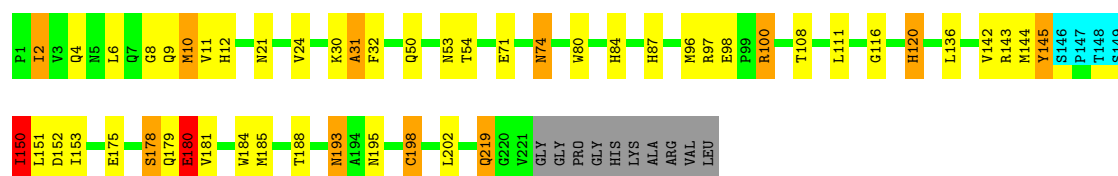
Chain B: 67% 23%



4.2.16 Score per residue for model 16

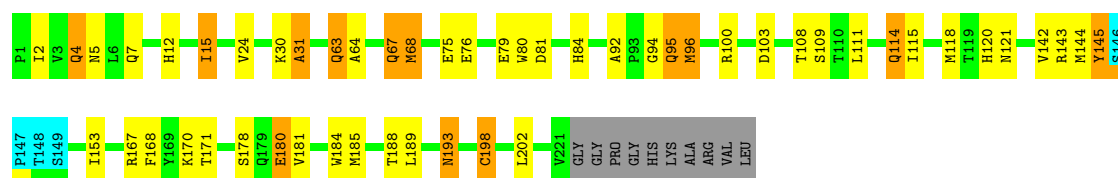
• Molecule 1: Capsid protein p24

Chain A: 72% 16% 5%



• Molecule 1: Capsid protein p24

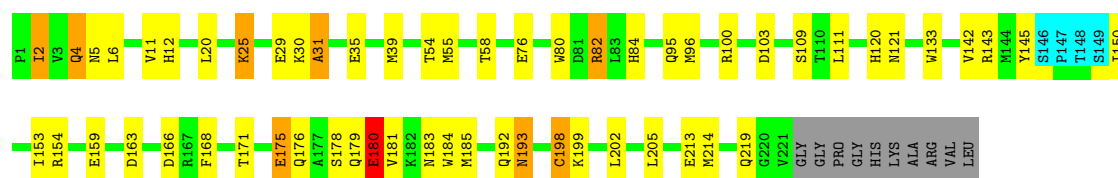
Chain B: 



4.2.17 Score per residue for model 17

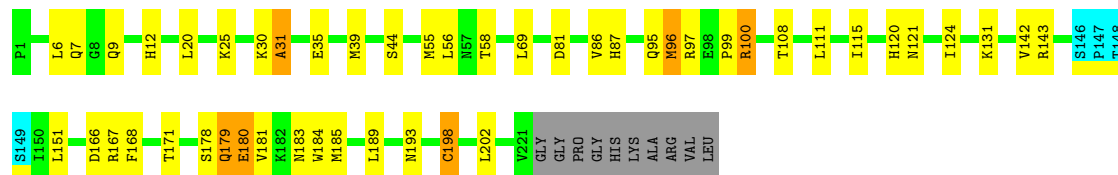
- Molecule 1: Capsid protein p24

Chain A: 



- Molecule 1: Capsid protein p24

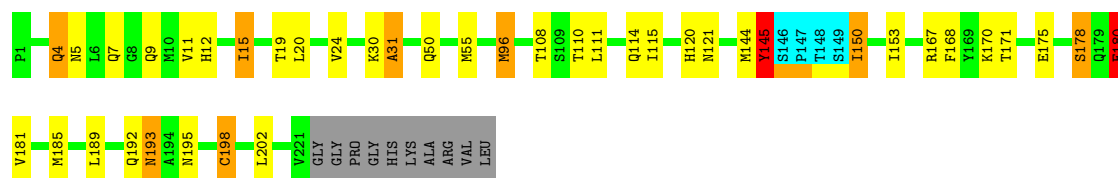
Chain B: 



4.2.18 Score per residue for model 18

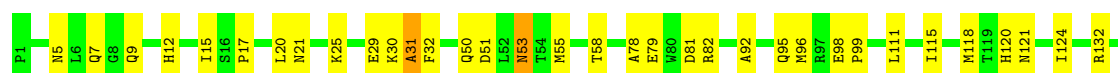
- Molecule 1: Capsid protein p24

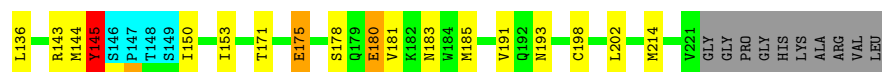
Chain A: 



- Molecule 1: Capsid protein p24

Chain B: 

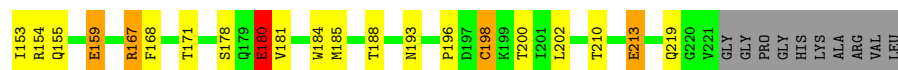




4.2.19 Score per residue for model 19

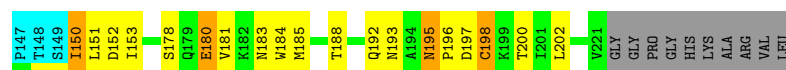
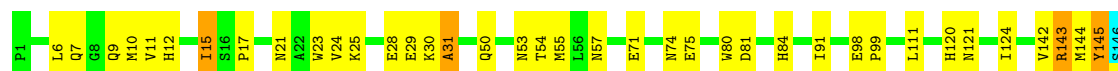
- Molecule 1: Capsid protein p24

Chain A: 70% 20% . . .



- Molecule 1: Capsid protein p24

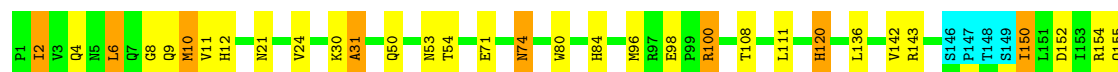
Chain B: 69% 21% . . .



4.2.20 Score per residue for model 20

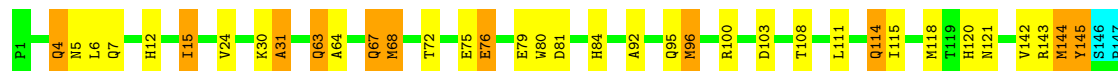
- Molecule 1: Capsid protein p24

Chain A: 75% 13% 5% . . .



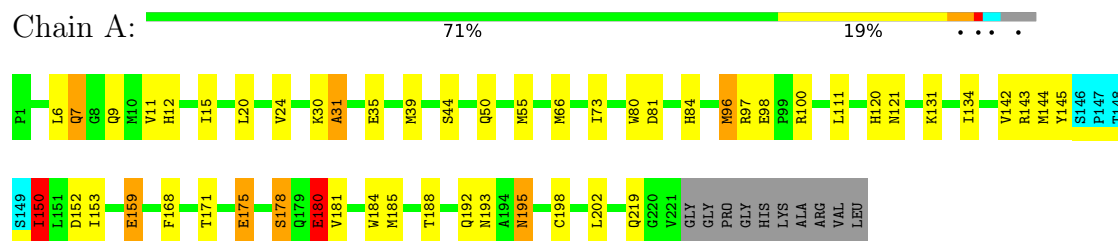
- Molecule 1: Capsid protein p24

Chain B: 72% 16% 6% . . .

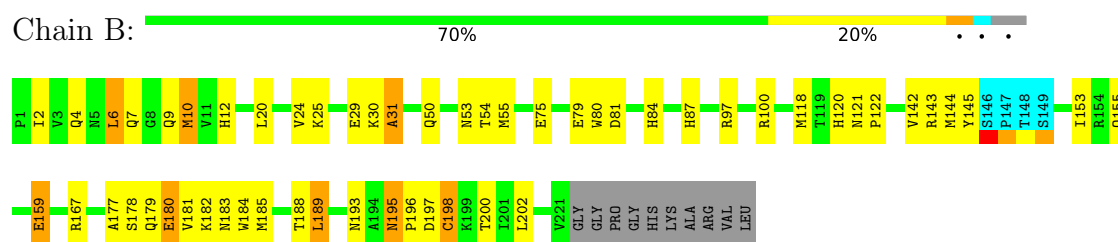


4.2.21 Score per residue for model 21

- Molecule 1: Capsid protein p24

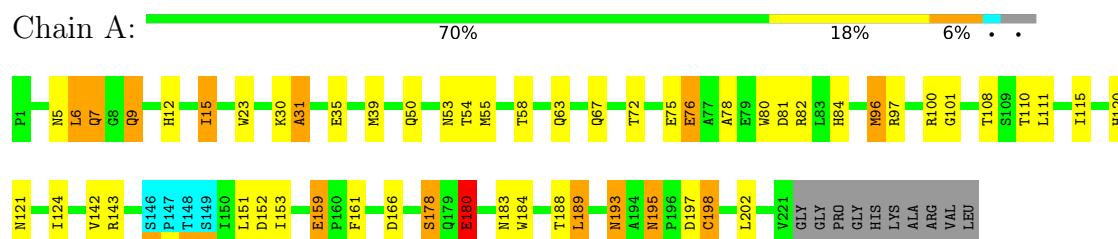


- Molecule 1: Capsid protein p24

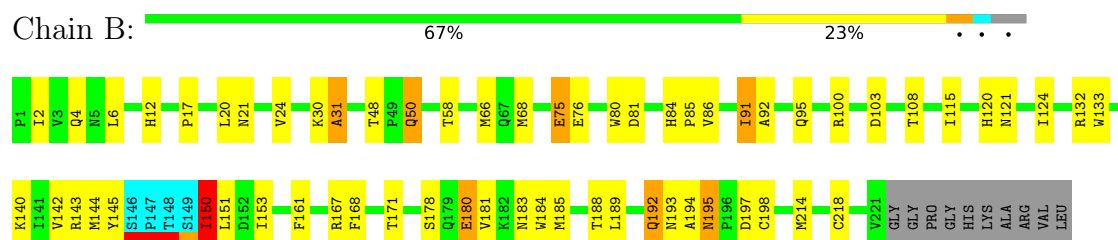


4.2.22 Score per residue for model 22

- Molecule 1: Capsid protein p24

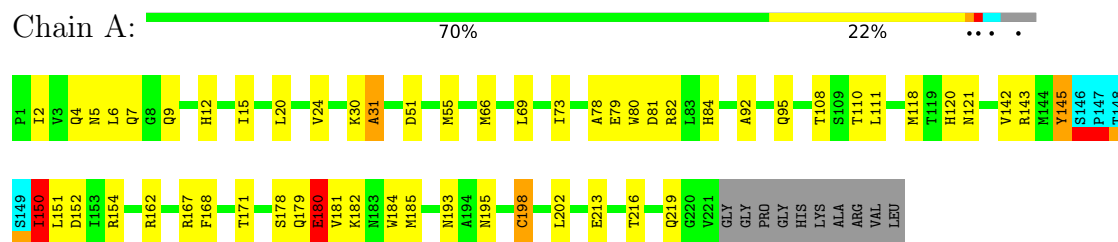


- Molecule 1: Capsid protein p24

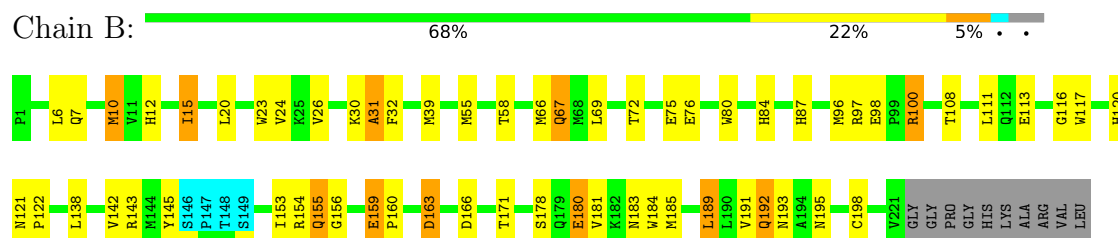


4.2.23 Score per residue for model 23

- Molecule 1: Capsid protein p24

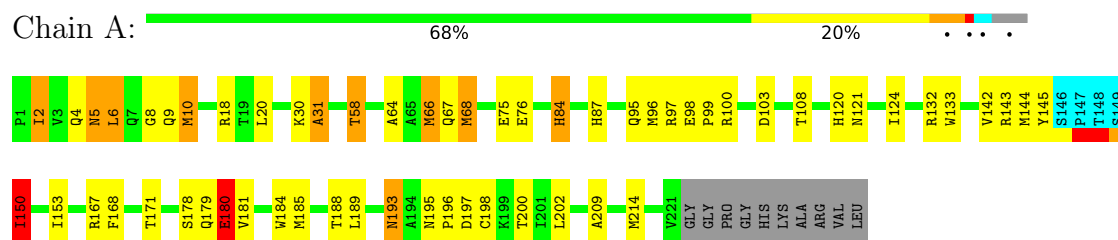


- Molecule 1: Capsid protein p24

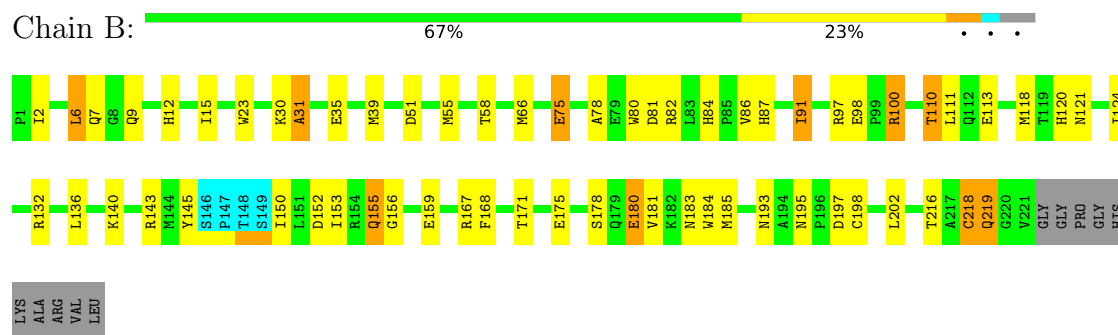


4.2.24 Score per residue for model 24

- Molecule 1: Capsid protein p24



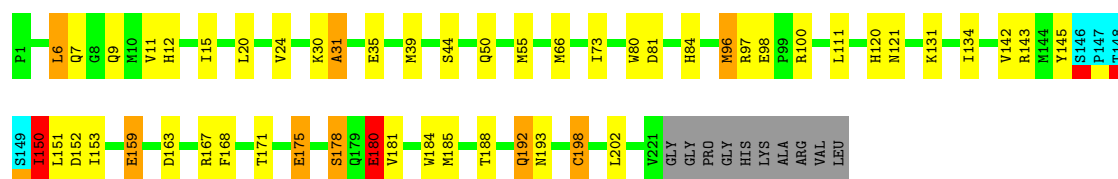
- Molecule 1: Capsid protein p24



4.2.25 Score per residue for model 25

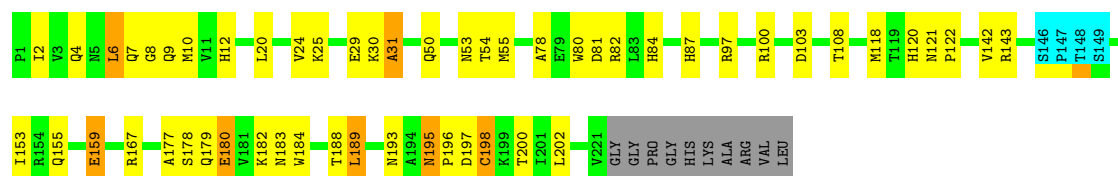
- Molecule 1: Capsid protein p24





- Molecule 1: Capsid protein p24

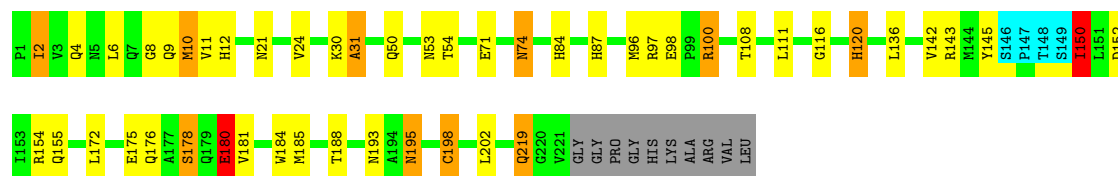
Chain B: 71% 20%



4.2.26 Score per residue for model 26

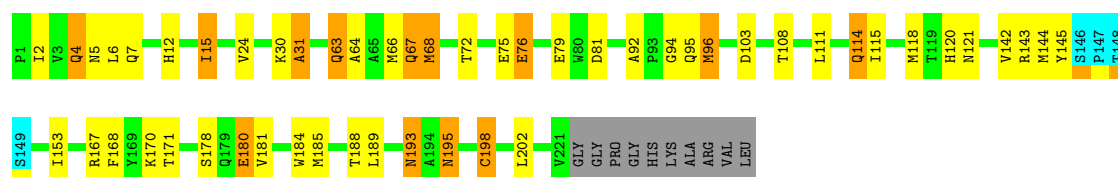
- Molecule 1: Capsid protein p24

Chain A: 73% 16%



- Molecule 1: Capsid protein p24

Chain B: 71% 17% 6%

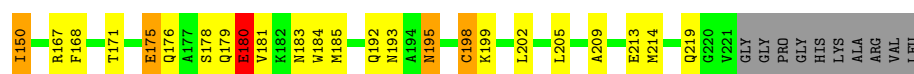


4.2.27 Score per residue for model 27

- Molecule 1: Capsid protein p24

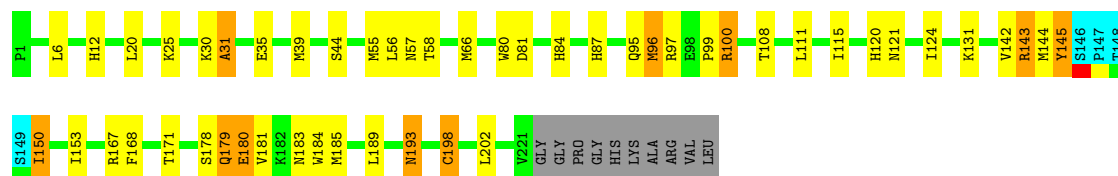
Chain A: 69% 21%





- Molecule 1: Capsid protein p24

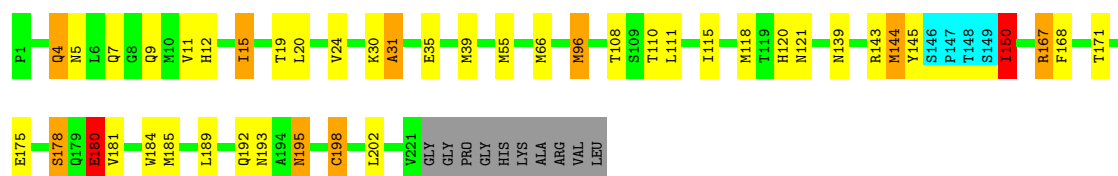
Chain B: 72% 17% . . .



4.2.28 Score per residue for model 28

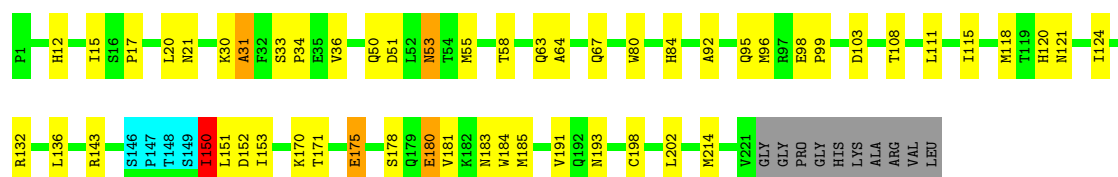
- Molecule 1: Capsid protein p24

Chain A: 75% 14% . . .



- Molecule 1: Capsid protein p24

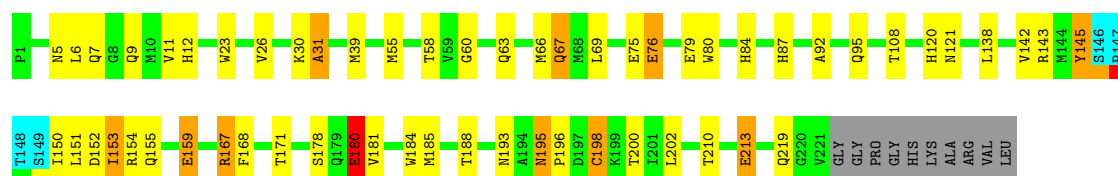
Chain B: 71% 21% . . .



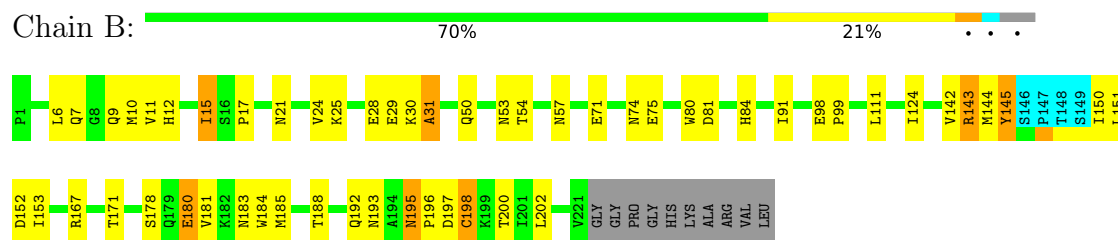
4.2.29 Score per residue for model 29

- Molecule 1: Capsid protein p24

Chain A: 69% 20% . . .

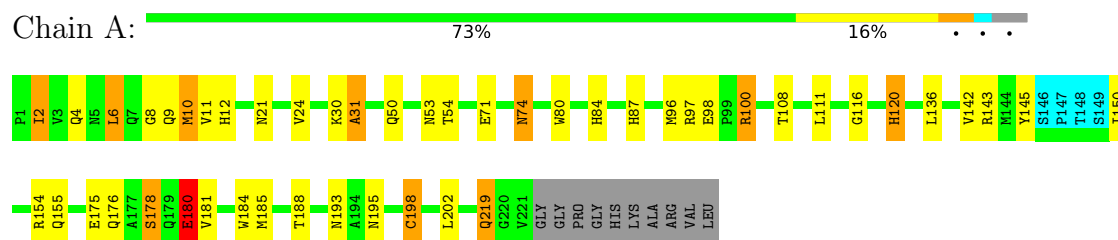


- Molecule 1: Capsid protein p24

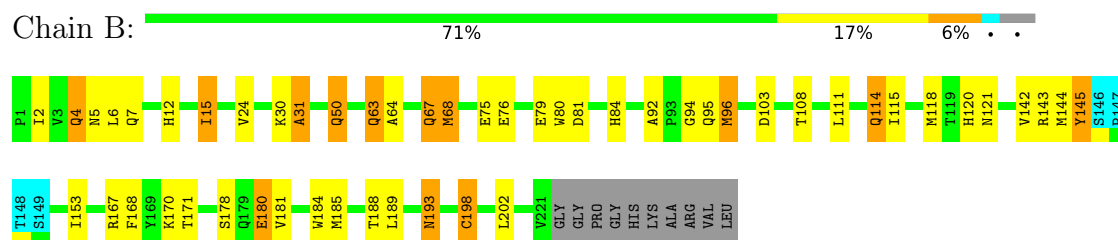


4.2.30 Score per residue for model 30

- Molecule 1: Capsid protein p24

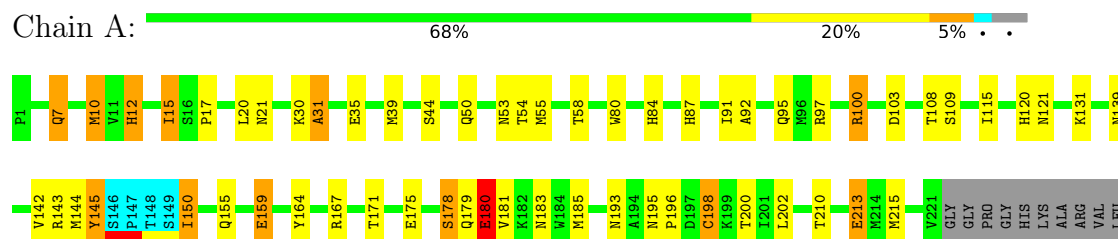


- Molecule 1: Capsid protein p24

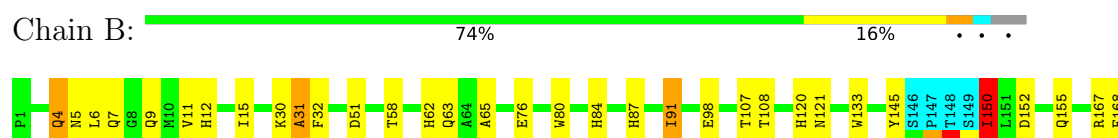


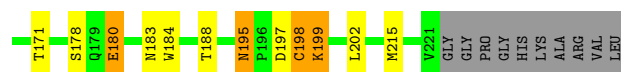
4.2.31 Score per residue for model 31

- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24

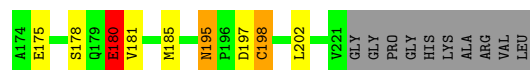




4.2.32 Score per residue for model 32

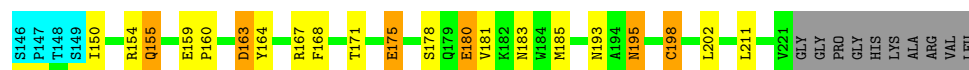
- Molecule 1: Capsid protein p24

Chain A: 75% 15% . . .



- Molecule 1: Capsid protein p24

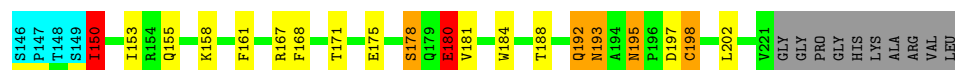
Chain B: 69% 19% 6% . .



4.2.33 Score per residue for model 33

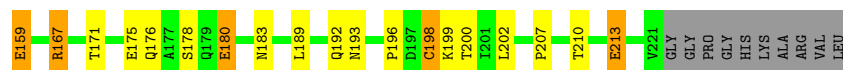
- Molecule 1: Capsid protein p24

Chain A: 70% 19% . . .



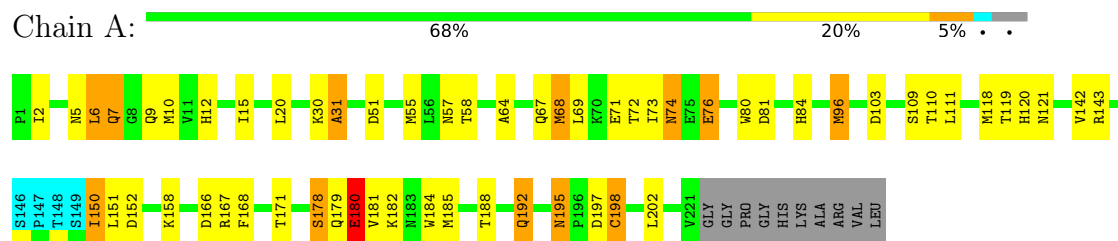
- Molecule 1: Capsid protein p24

Chain B: 71% 19% . . .

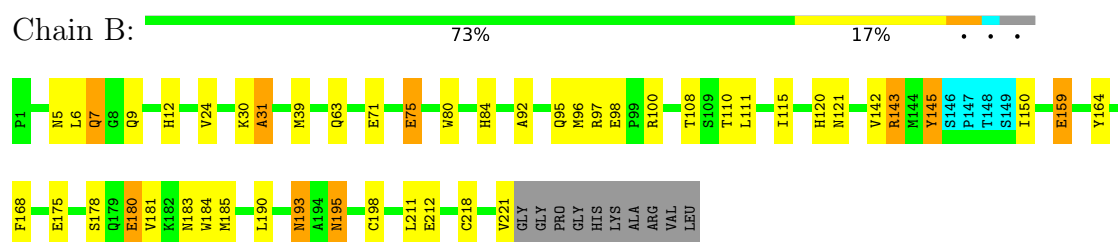


4.2.34 Score per residue for model 34

- Molecule 1: Capsid protein p24

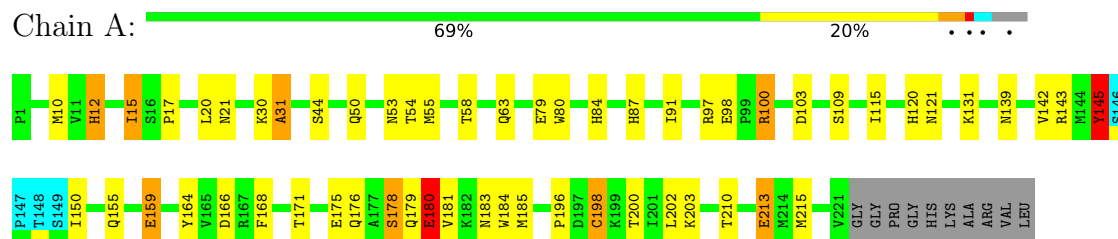


- Molecule 1: Capsid protein p24

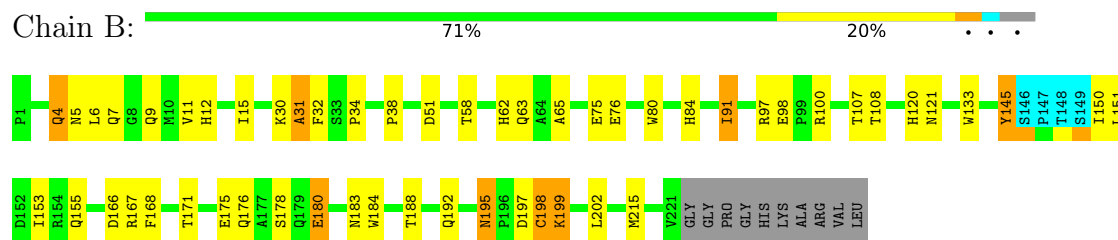


4.2.35 Score per residue for model 35

- Molecule 1: Capsid protein p24

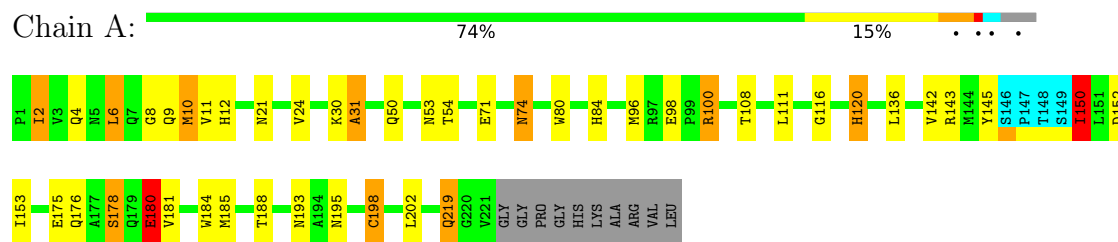


- Molecule 1: Capsid protein p24

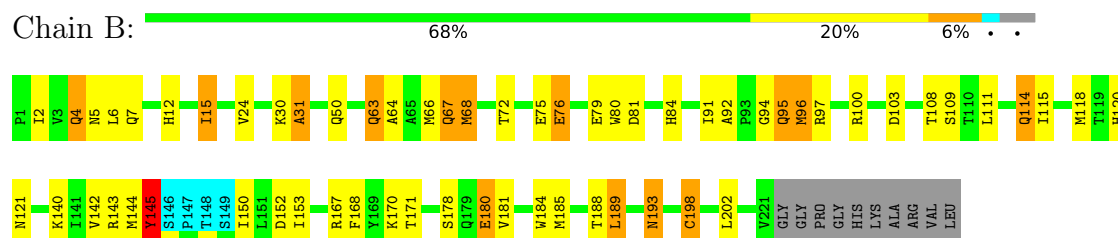


4.2.36 Score per residue for model 36

- Molecule 1: Capsid protein p24

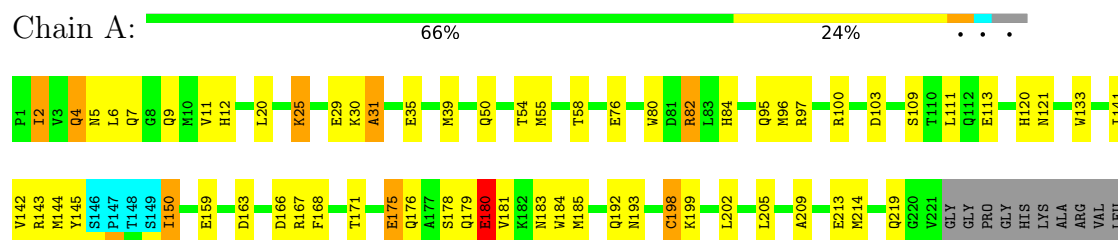


- Molecule 1: Capsid protein p24

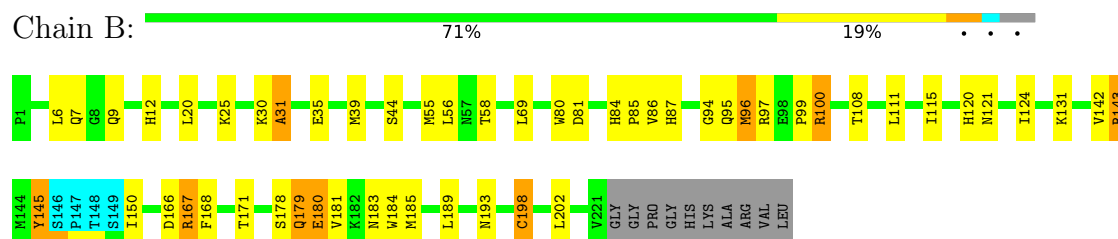


4.2.37 Score per residue for model 37

- Molecule 1: Capsid protein p24

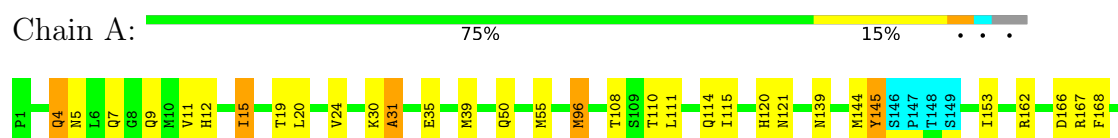


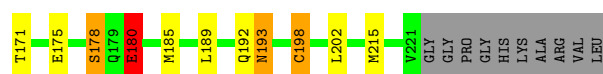
- Molecule 1: Capsid protein p24



4.2.38 Score per residue for model 38

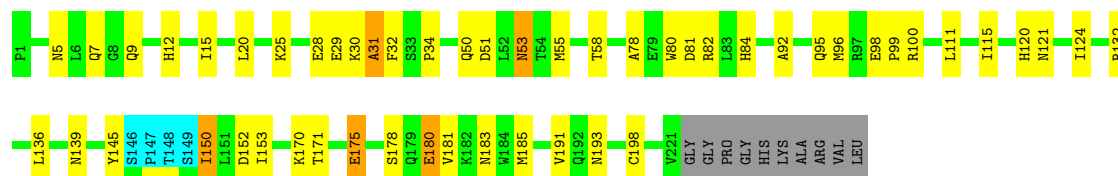
- Molecule 1: Capsid protein p24





- Molecule 1: Capsid protein p24

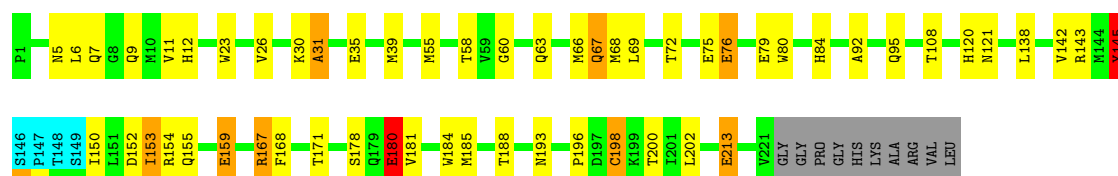
Chain B: 71% 20% . . .



4.2.39 Score per residue for model 39

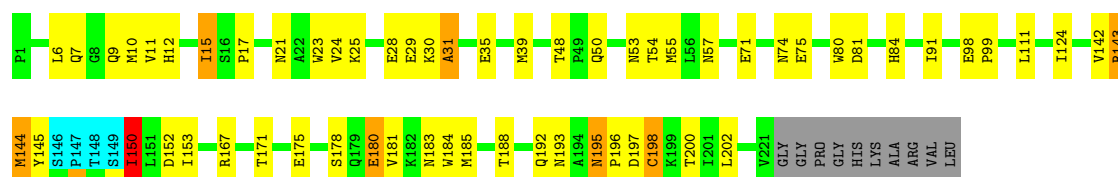
- Molecule 1: Capsid protein p24

Chain A: 70% 20% . . .



- Molecule 1: Capsid protein p24

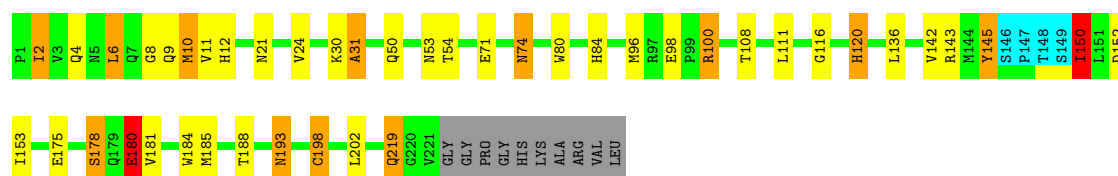
Chain B: 68% 23% . . .



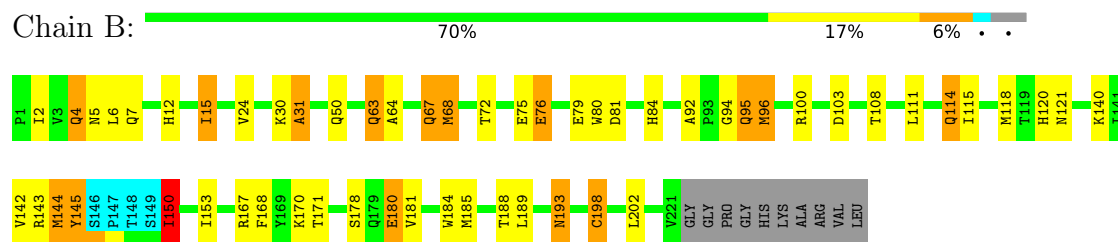
4.2.40 Score per residue for model 40

- Molecule 1: Capsid protein p24

Chain A: 75% 13% 5% . . .

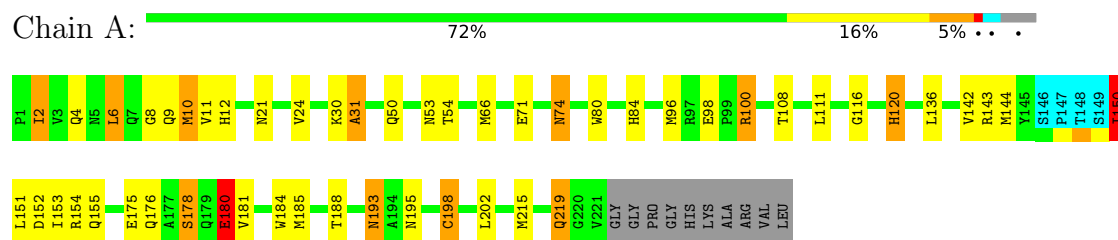


- Molecule 1: Capsid protein p24

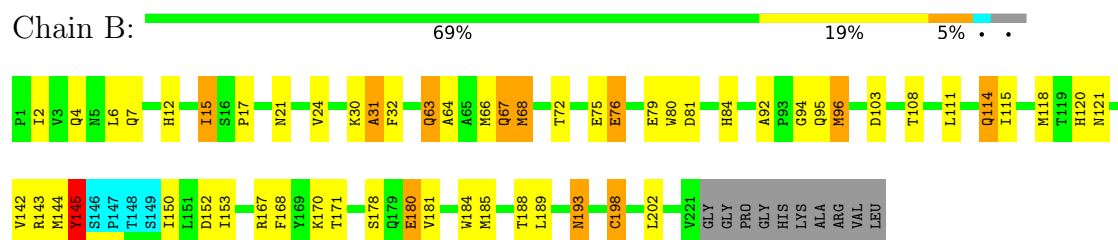


4.2.41 Score per residue for model 41

- Molecule 1: Capsid protein p24

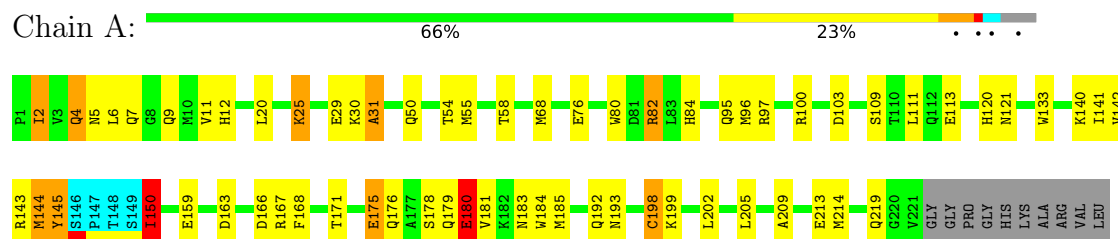


- Molecule 1: Capsid protein p24

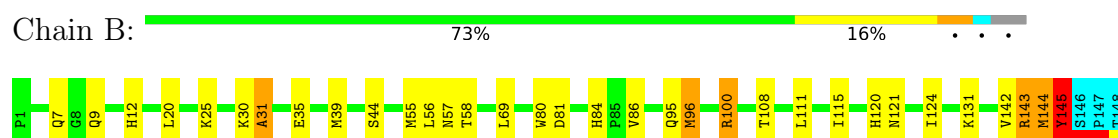


4.2.42 Score per residue for model 42

- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24

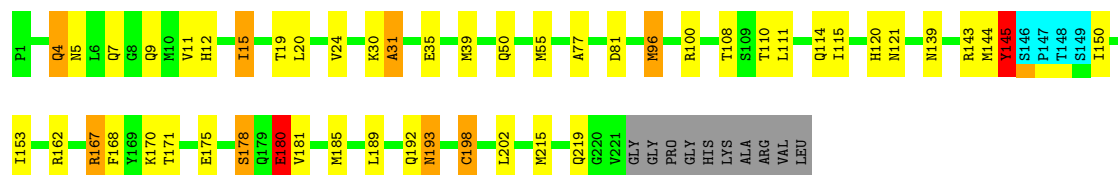




4.2.43 Score per residue for model 43

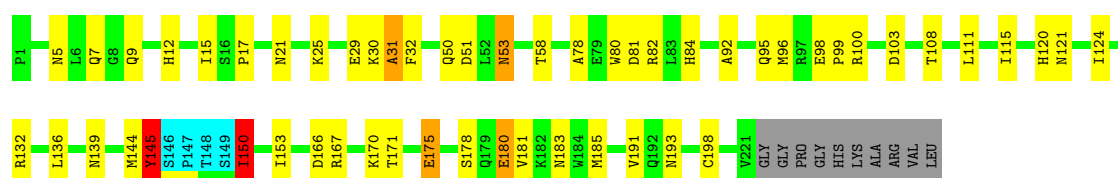
- Molecule 1: Capsid protein p24

Chain A: 72% 17% . . .



- Molecule 1: Capsid protein p24

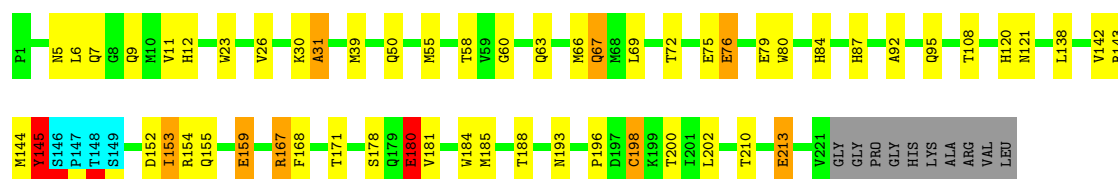
Chain B: 71% 21% . . .



4.2.44 Score per residue for model 44

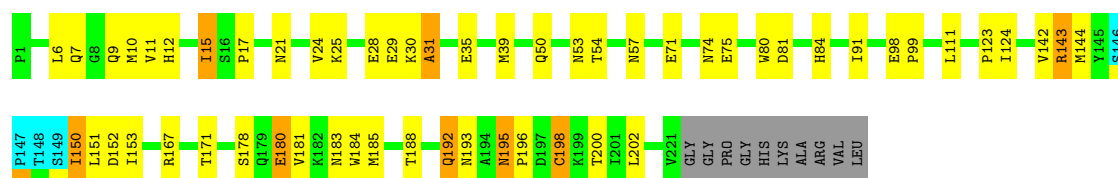
- Molecule 1: Capsid protein p24

Chain A: 69% 20% . . .



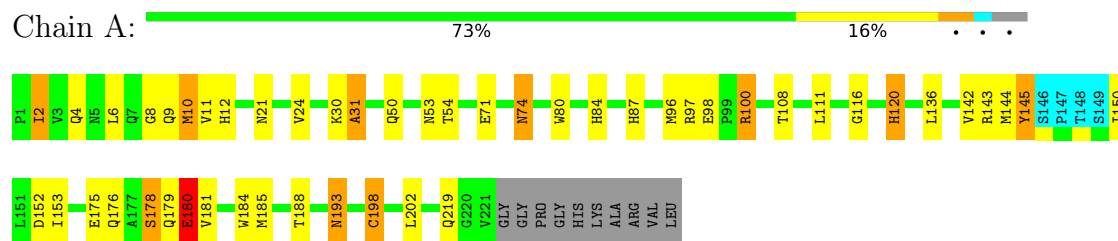
- Molecule 1: Capsid protein p24

Chain B: 70% 21% . . .

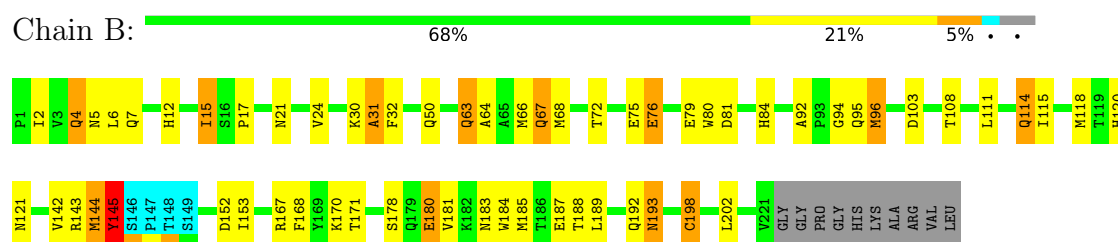


4.2.45 Score per residue for model 45

- Molecule 1: Capsid protein p24

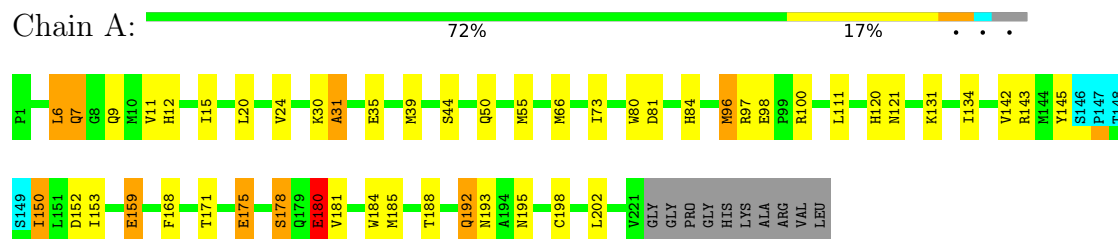


- Molecule 1: Capsid protein p24

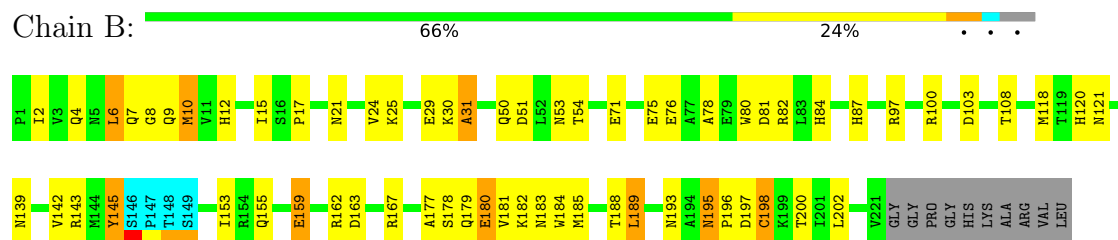


4.2.46 Score per residue for model 46

- Molecule 1: Capsid protein p24

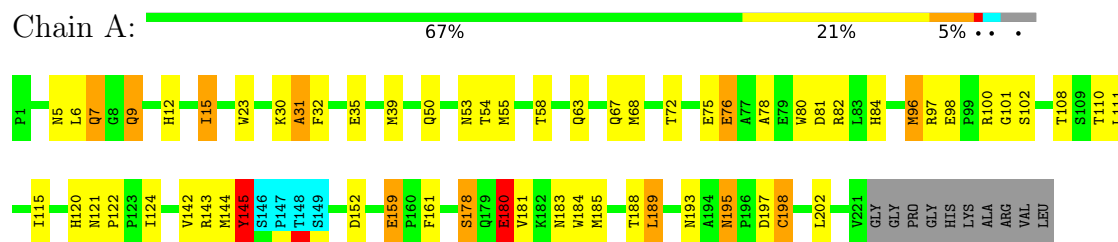


- Molecule 1: Capsid protein p24

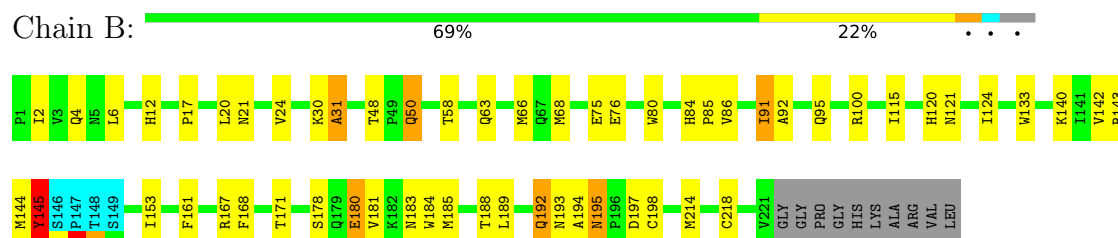


4.2.47 Score per residue for model 47

- Molecule 1: Capsid protein p24

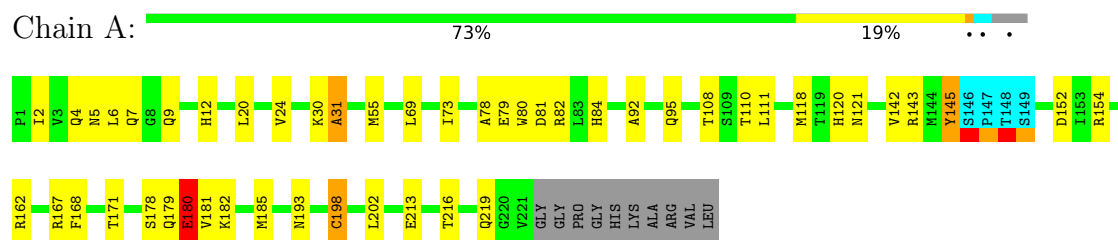


- Molecule 1: Capsid protein p24

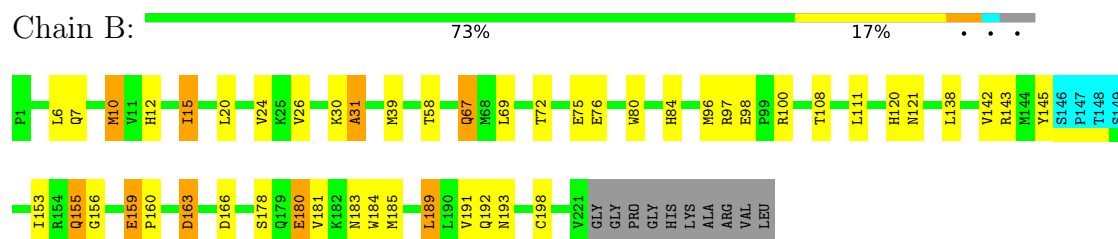


4.2.48 Score per residue for model 48

- Molecule 1: Capsid protein p24

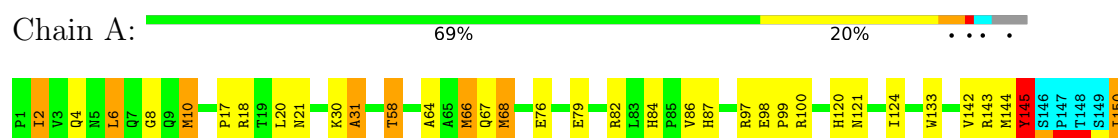


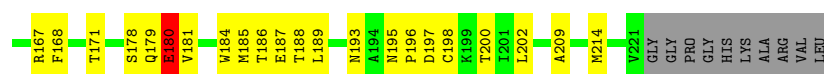
- Molecule 1: Capsid protein p24



4.2.49 Score per residue for model 49

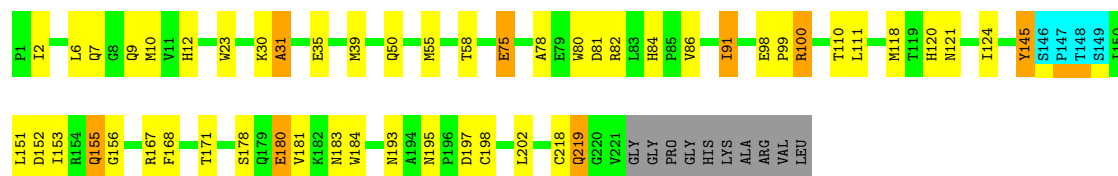
- Molecule 1: Capsid protein p24





• Molecule 1: Capsid protein p24

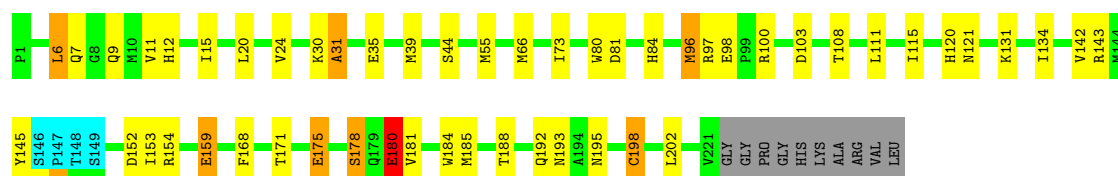
Chain B: 71% 19% . . .



4.2.50 Score per residue for model 50

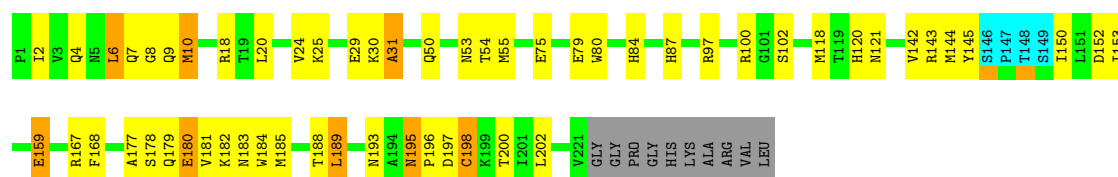
• Molecule 1: Capsid protein p24

Chain A: 71% 19% . . .



• Molecule 1: Capsid protein p24

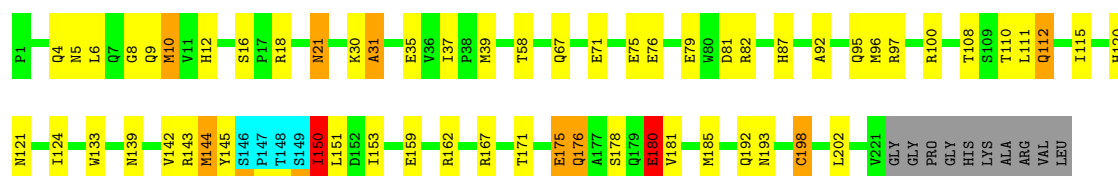
Chain B: 69% 21% . . .



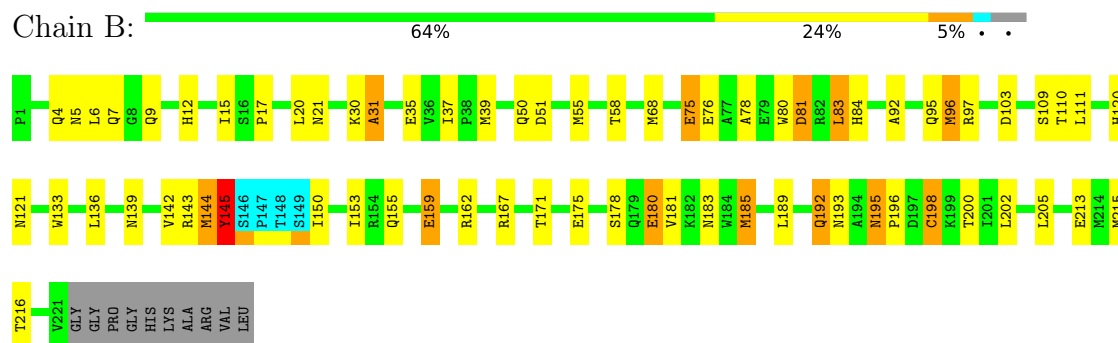
4.2.51 Score per residue for model 51

• Molecule 1: Capsid protein p24

Chain A: 68% 22% . . .

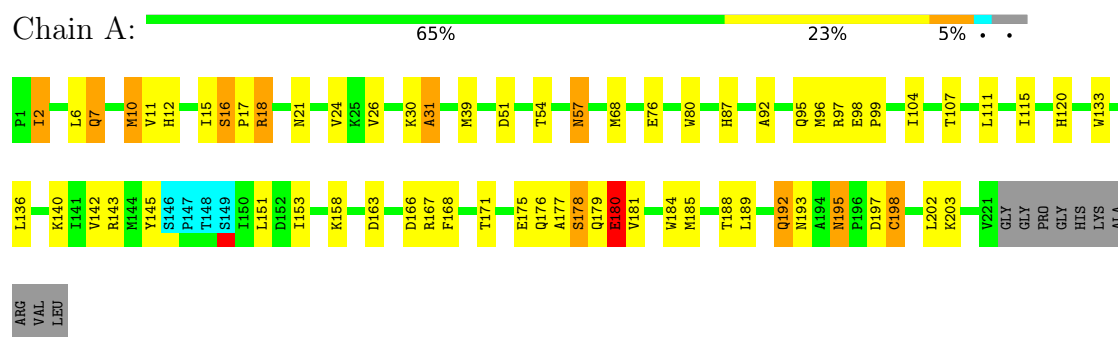


• Molecule 1: Capsid protein p24

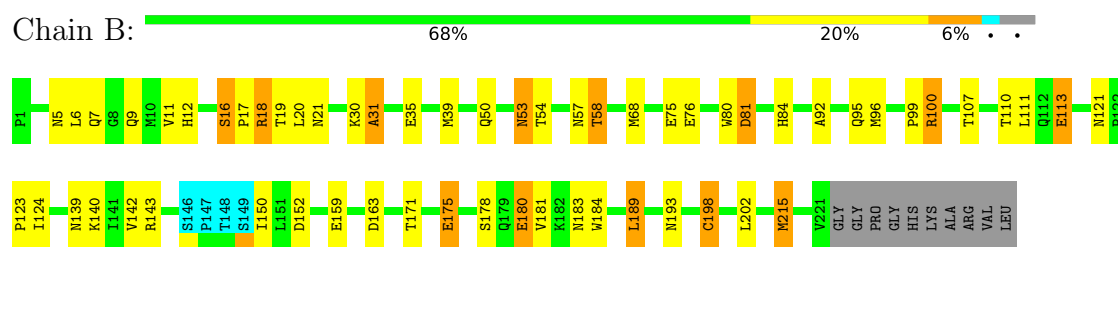


4.2.52 Score per residue for model 52

- Molecule 1: Capsid protein p24

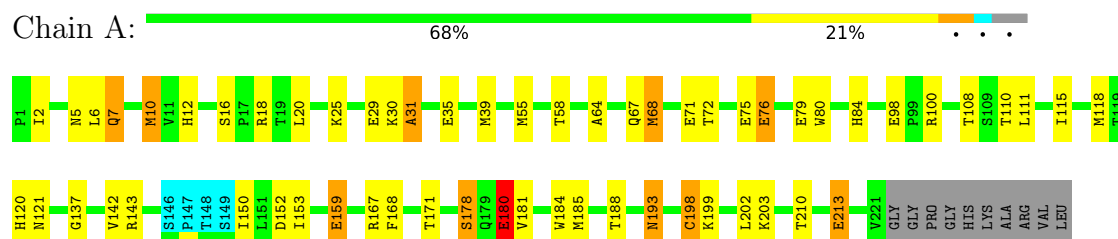


- Molecule 1: Capsid protein p24

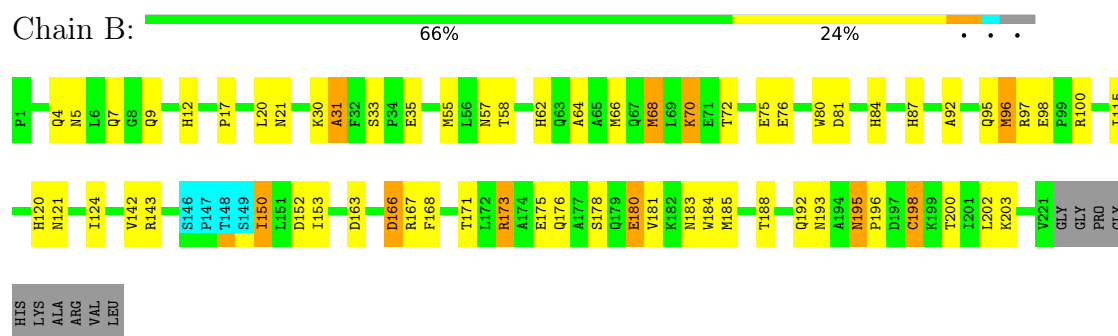


4.2.53 Score per residue for model 53

- Molecule 1: Capsid protein p24

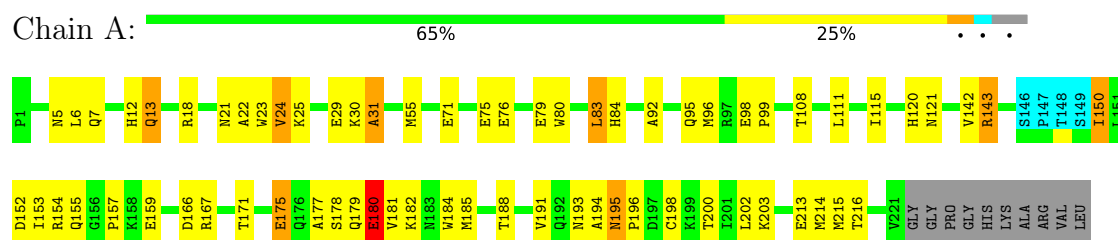


- Molecule 1: Capsid protein p24

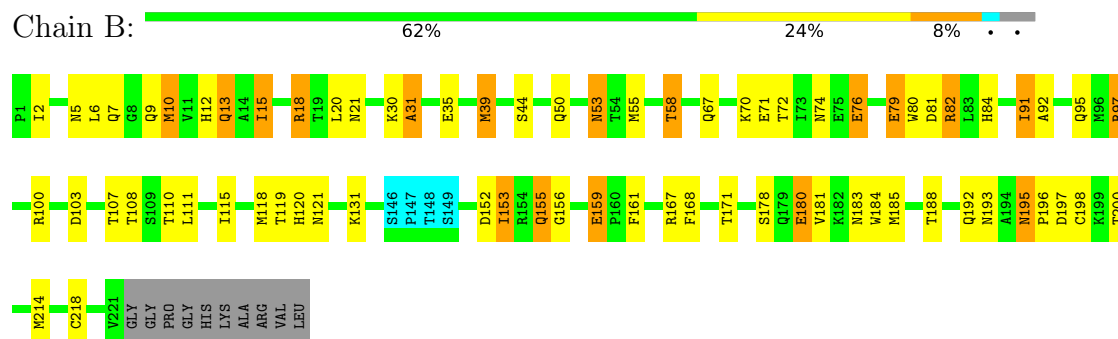


4.2.54 Score per residue for model 54

- Molecule 1: Capsid protein p24

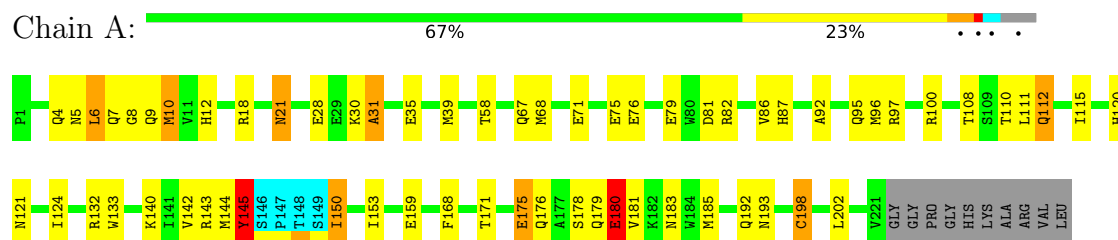


- Molecule 1: Capsid protein p24

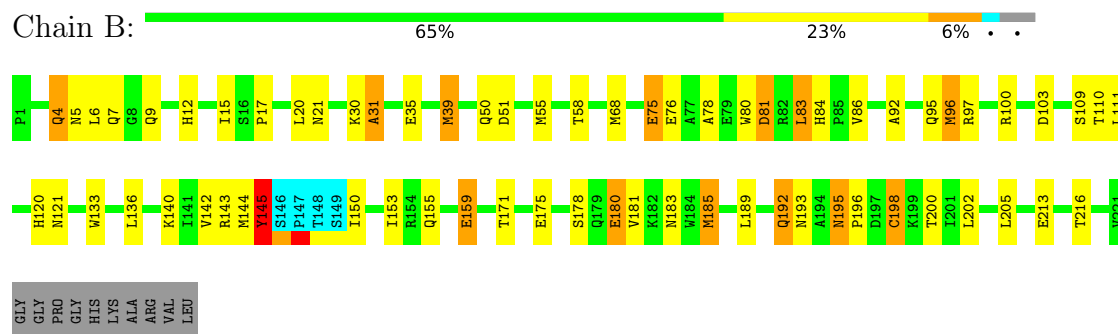


4.2.55 Score per residue for model 55

- Molecule 1: Capsid protein p24

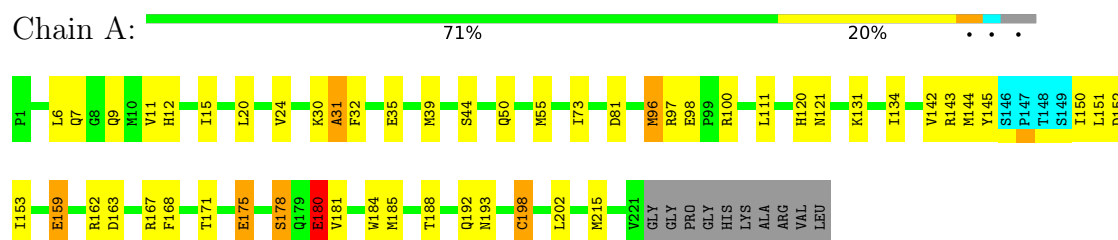


- Molecule 1: Capsid protein p24

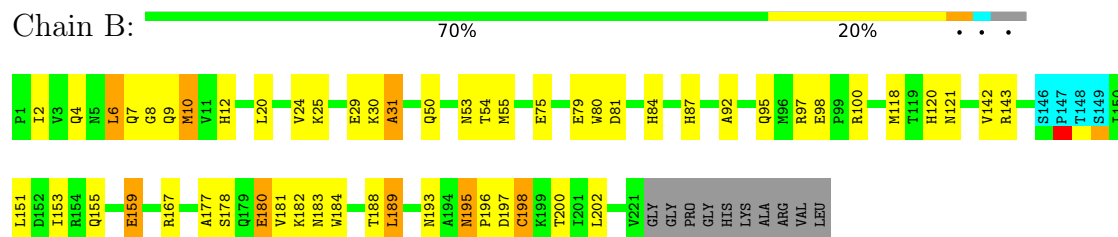


4.2.56 Score per residue for model 56

- Molecule 1: Capsid protein p24

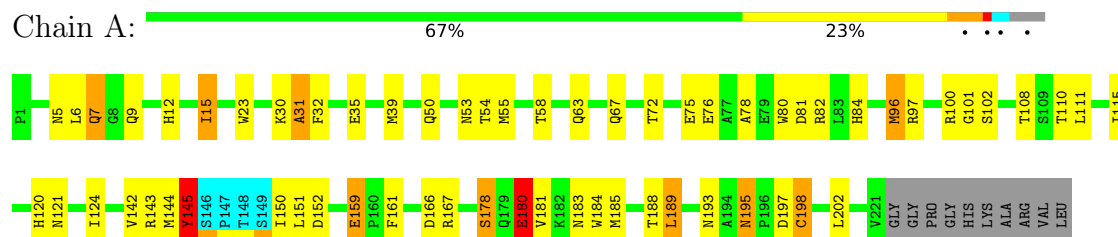


- Molecule 1: Capsid protein p24

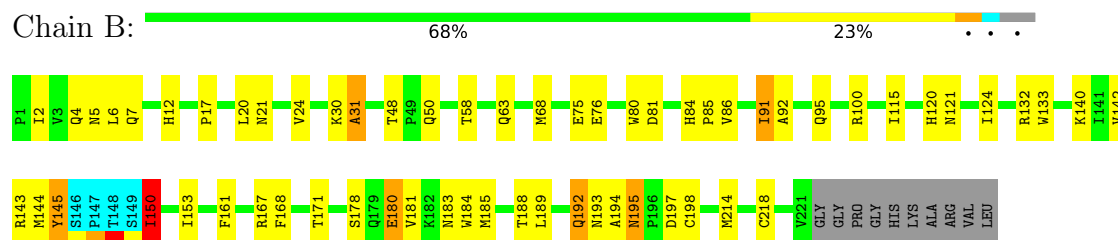


4.2.57 Score per residue for model 57

- Molecule 1: Capsid protein p24

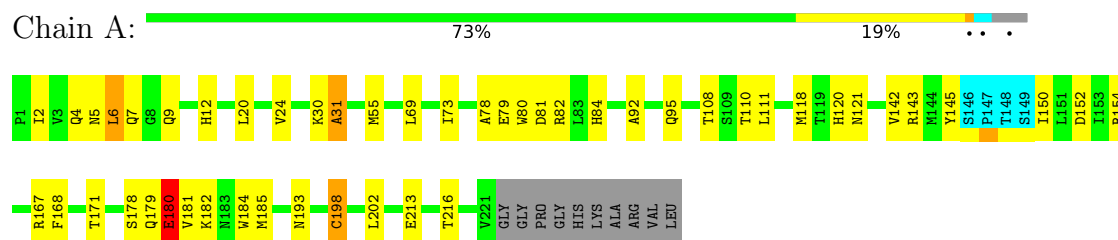


- Molecule 1: Capsid protein p24

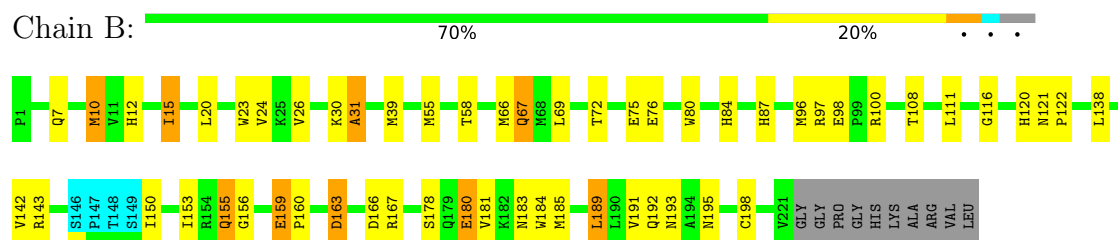


4.2.58 Score per residue for model 58

- Molecule 1: Capsid protein p24

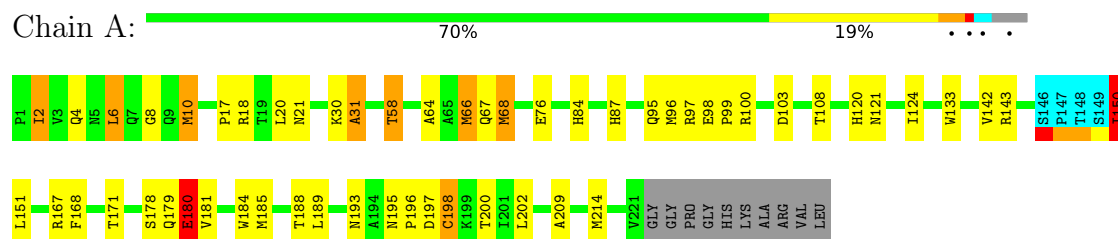


- Molecule 1: Capsid protein p24

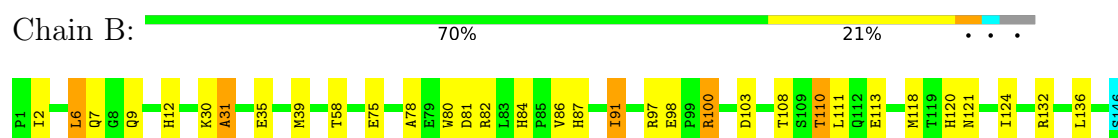


4.2.59 Score per residue for model 59

- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24

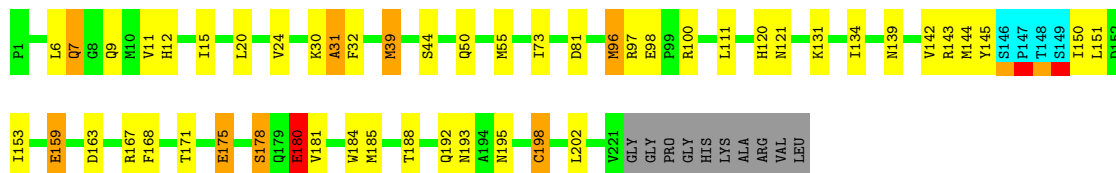




4.2.60 Score per residue for model 60

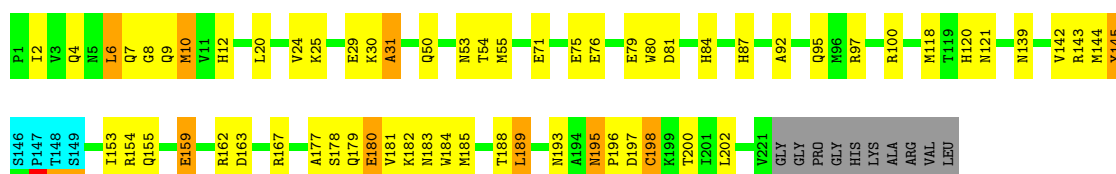
- Molecule 1: Capsid protein p24

Chain A: 72% 18% . . .



- Molecule 1: Capsid protein p24

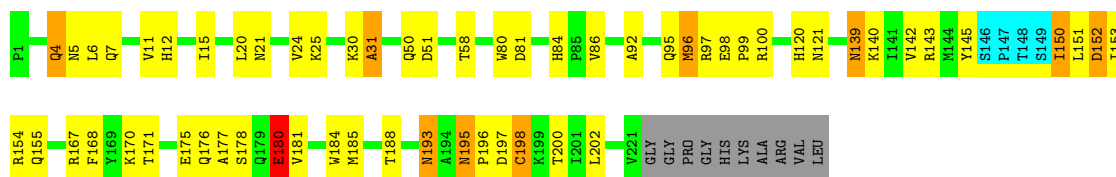
Chain B: 67% 23% . . .



4.2.61 Score per residue for model 61

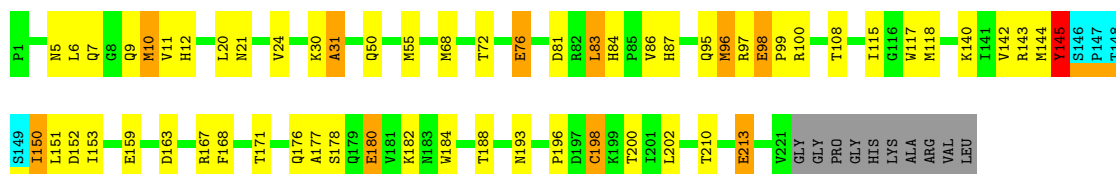
- Molecule 1: Capsid protein p24

Chain A: 68% 22% . . .



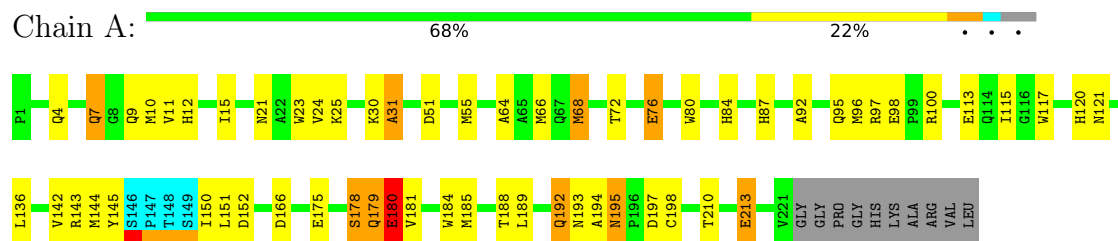
- Molecule 1: Capsid protein p24

Chain B: 68% 21% . . .

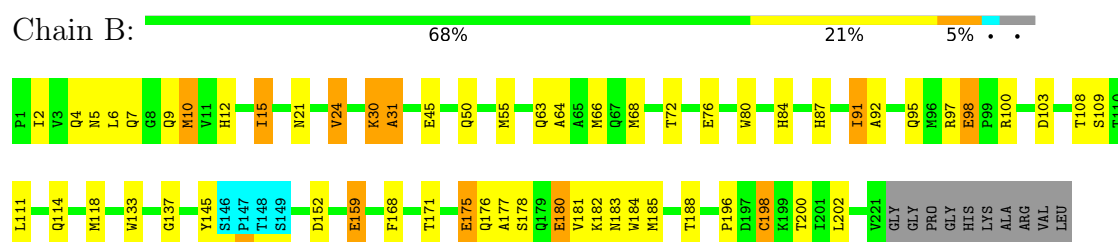


4.2.62 Score per residue for model 62

- Molecule 1: Capsid protein p24

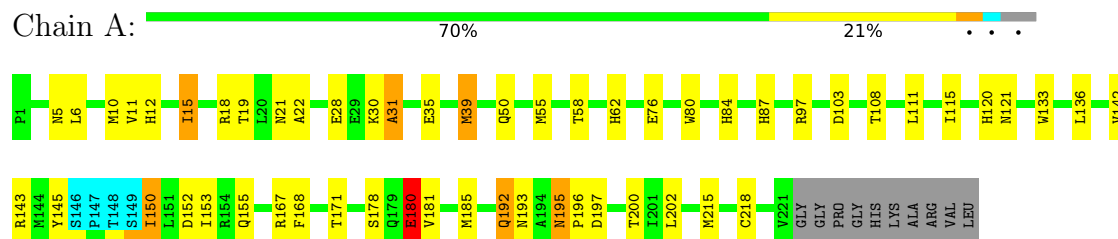


- Molecule 1: Capsid protein p24

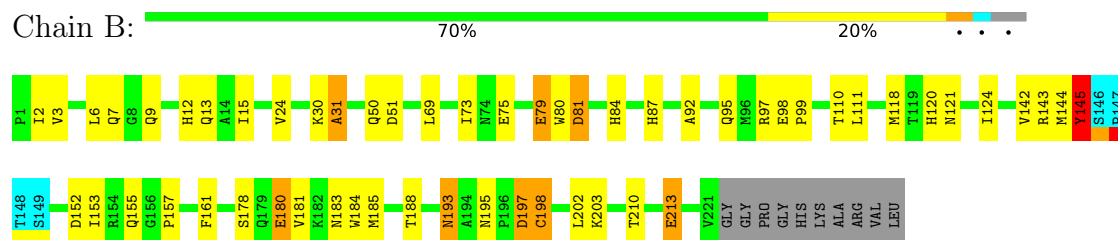


4.2.63 Score per residue for model 63

- Molecule 1: Capsid protein p24

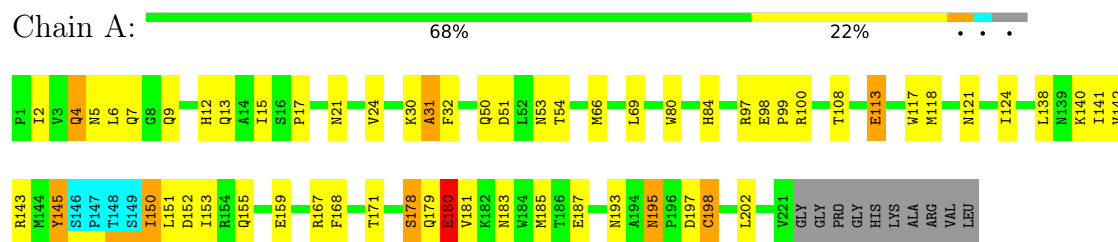


- Molecule 1: Capsid protein p24

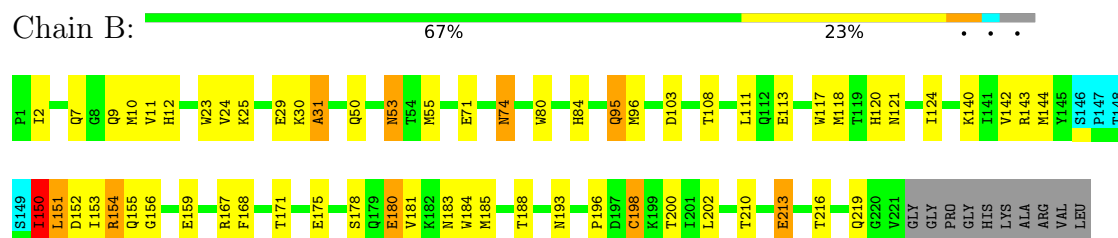


4.2.64 Score per residue for model 64

- Molecule 1: Capsid protein p24

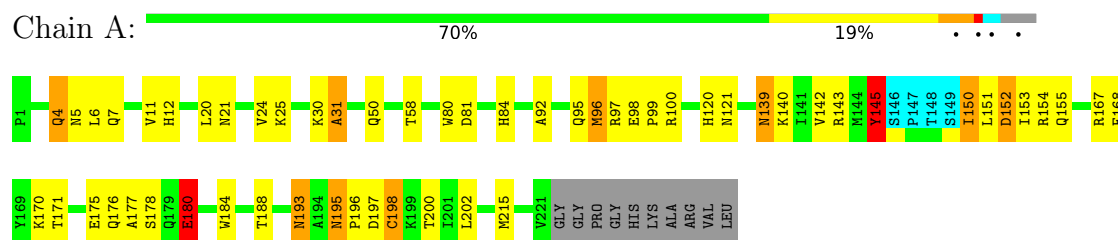


- Molecule 1: Capsid protein p24

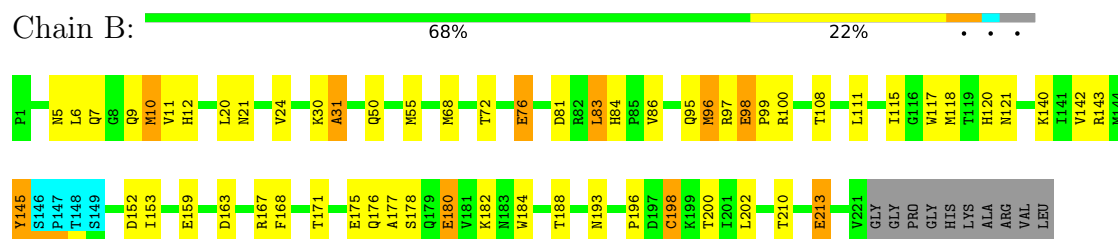


4.2.65 Score per residue for model 65

- Molecule 1: Capsid protein p24

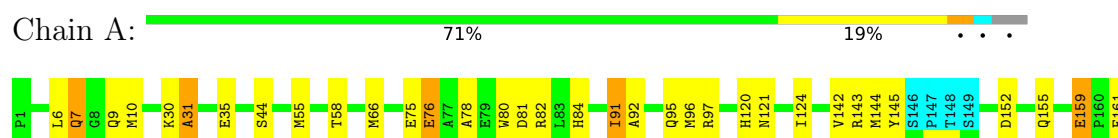


- Molecule 1: Capsid protein p24



4.2.66 Score per residue for model 66

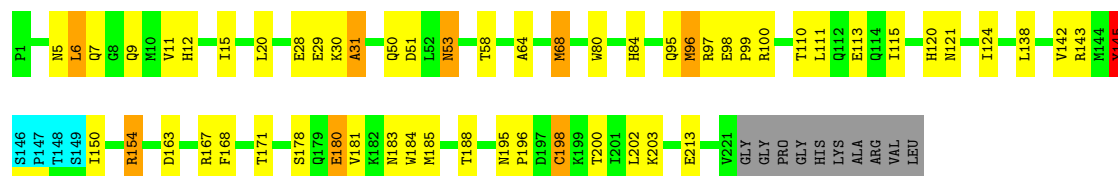
- Molecule 1: Capsid protein p24





- Molecule 1: Capsid protein p24

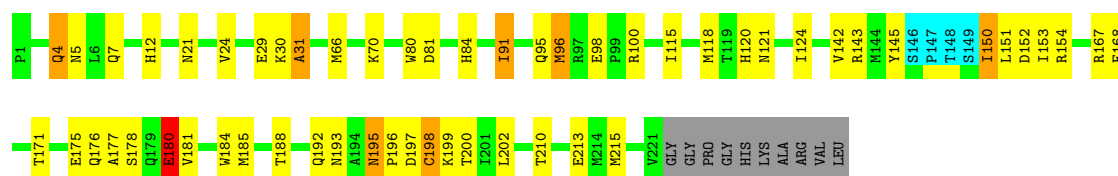
Chain B: 69% 21% . . .



4.2.67 Score per residue for model 67

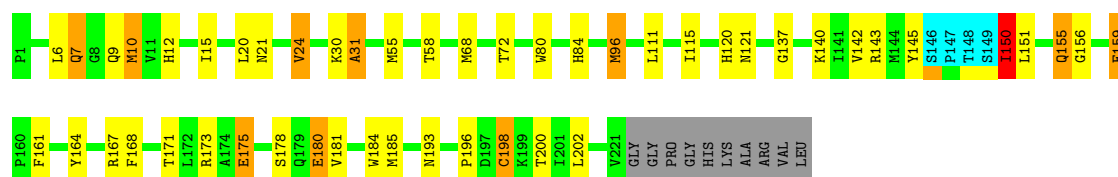
- Molecule 1: Capsid protein p24

Chain A: 70% 21% . . .



- Molecule 1: Capsid protein p24

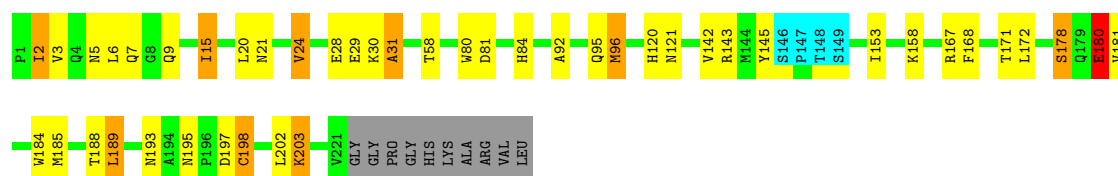
Chain B: 73% 16% . . .



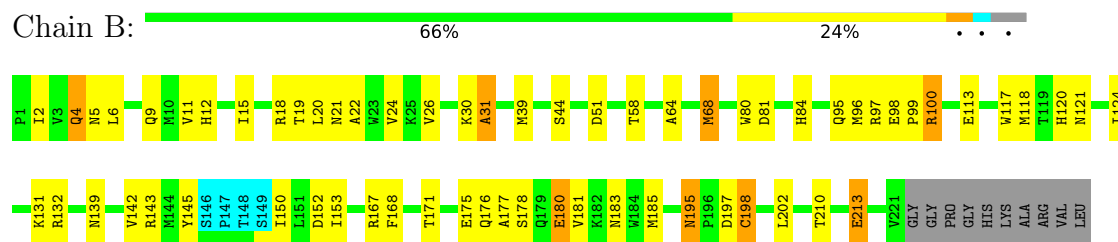
4.2.68 Score per residue for model 68

- Molecule 1: Capsid protein p24

Chain A: 74% 15% . . .

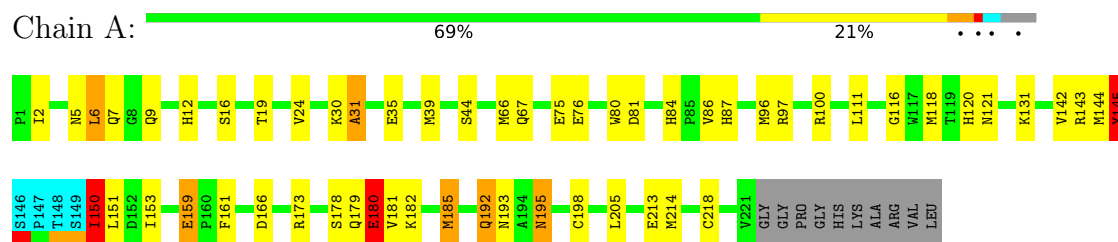


- Molecule 1: Capsid protein p24

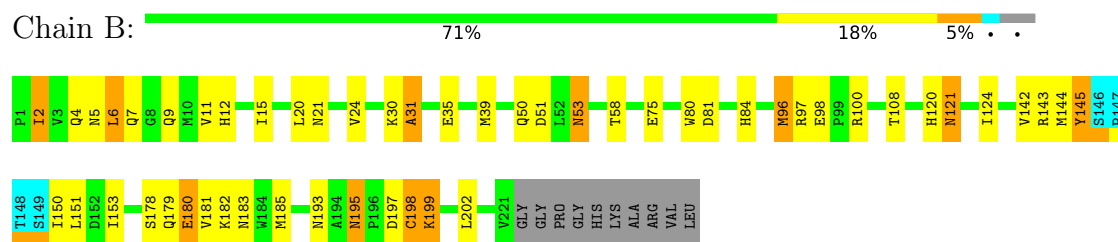


4.2.69 Score per residue for model 69

- Molecule 1: Capsid protein p24

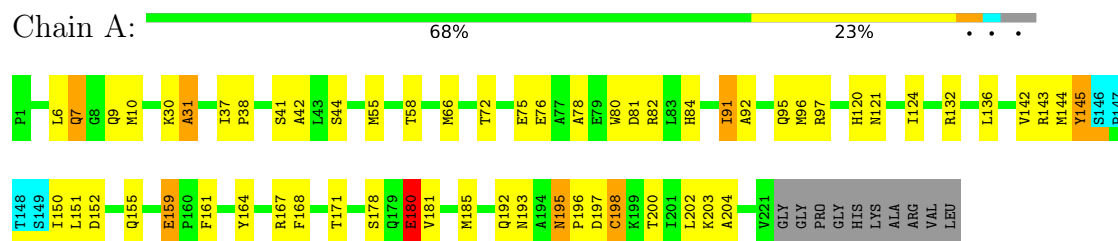


- Molecule 1: Capsid protein p24

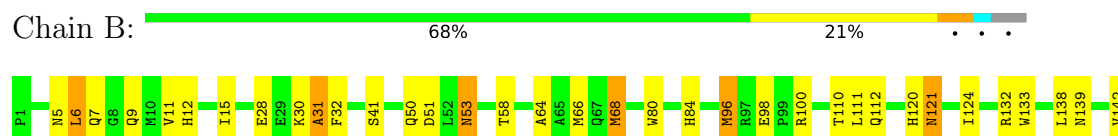


4.2.70 Score per residue for model 70

- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24





4.2.71 Score per residue for model 71

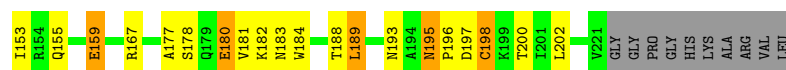
- Molecule 1: Capsid protein p24

Chain A: 71% 19%



- Molecule 1: Capsid protein p24

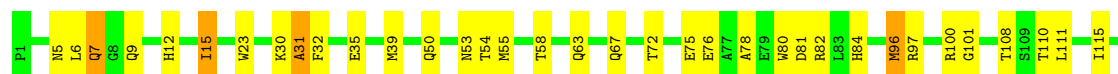
Chain B: 71% 20%



4.2.72 Score per residue for model 72

- Molecule 1: Capsid protein p24

Chain A: 67% 22%



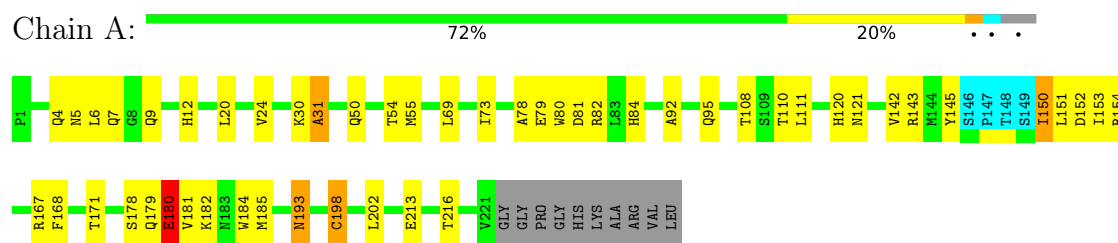
- Molecule 1: Capsid protein p24

Chain B: 68% 24%

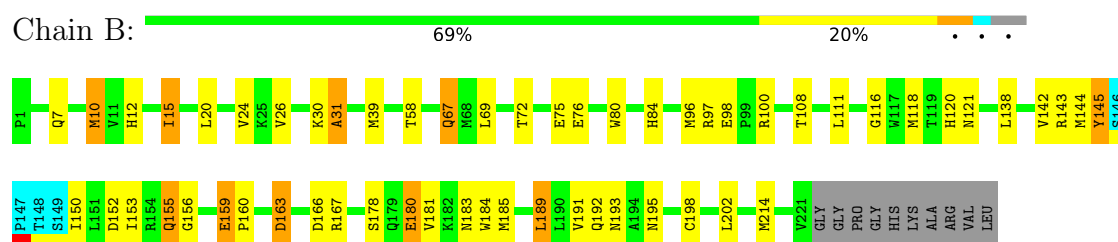


4.2.73 Score per residue for model 73

- Molecule 1: Capsid protein p24

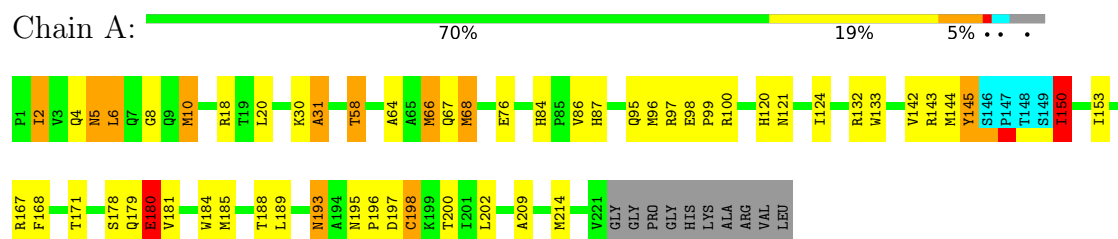


- Molecule 1: Capsid protein p24

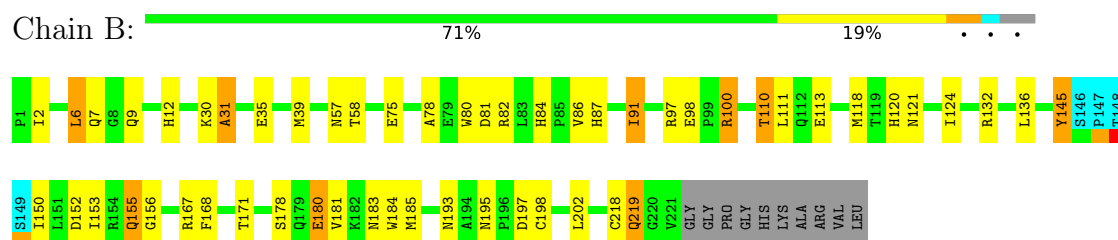


4.2.74 Score per residue for model 74

- Molecule 1: Capsid protein p24

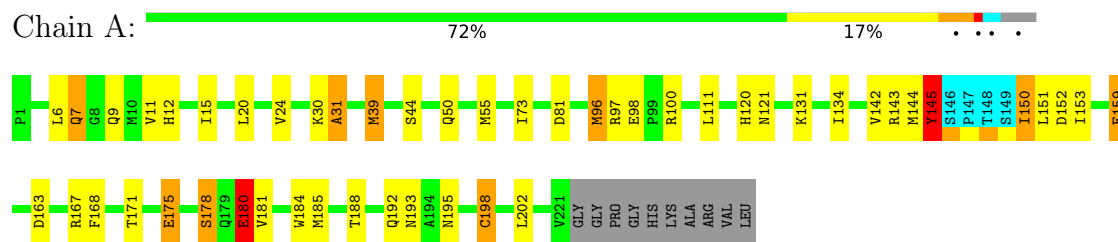


- Molecule 1: Capsid protein p24

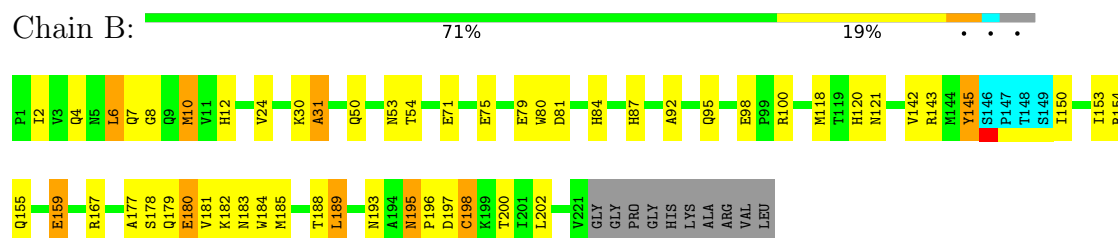


4.2.75 Score per residue for model 75

- Molecule 1: Capsid protein p24

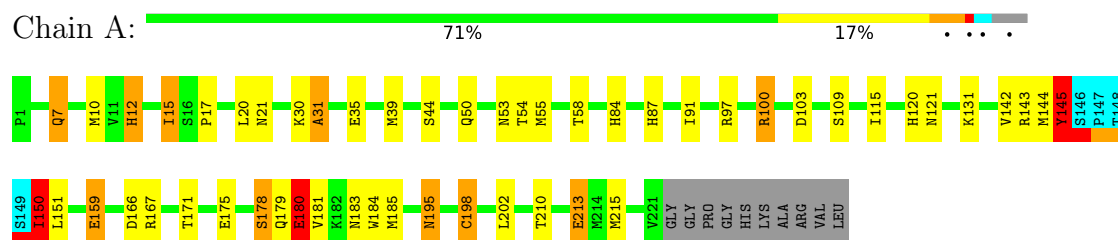


- Molecule 1: Capsid protein p24

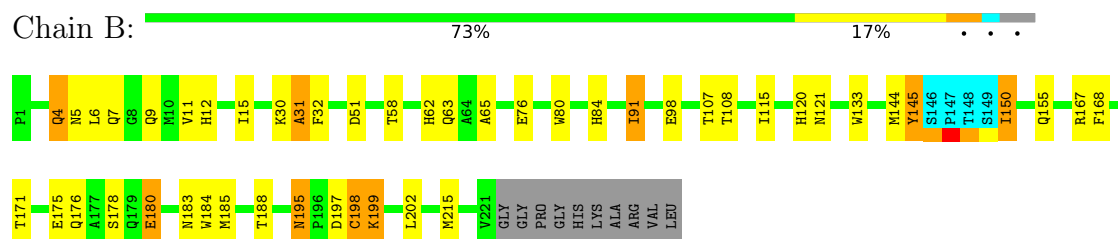


4.2.76 Score per residue for model 76

- Molecule 1: Capsid protein p24

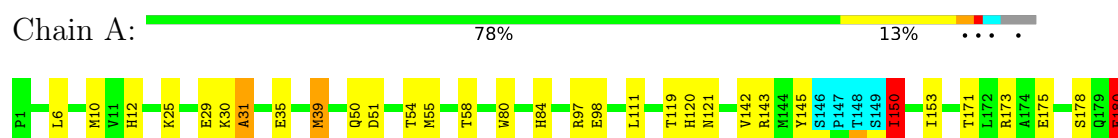


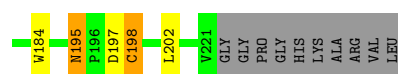
- Molecule 1: Capsid protein p24



4.2.77 Score per residue for model 77

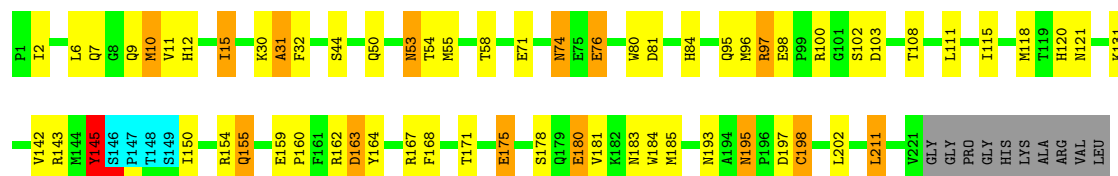
- Molecule 1: Capsid protein p24





• Molecule 1: Capsid protein p24

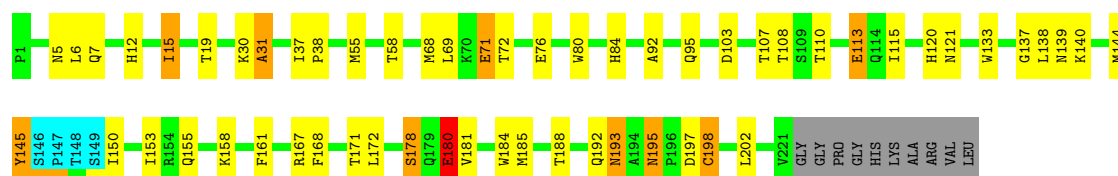
Chain B: 66% 21% 6% . . .



4.2.78 Score per residue for model 78

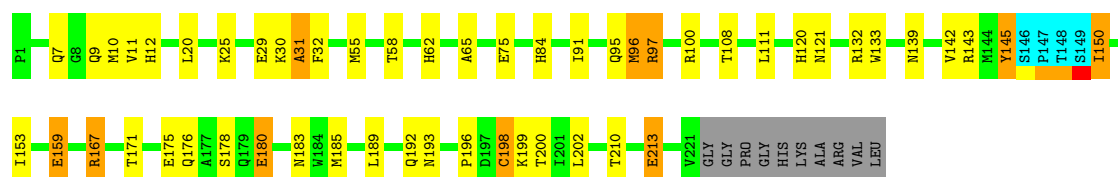
• Molecule 1: Capsid protein p24

Chain A: 69% 20% . . .



• Molecule 1: Capsid protein p24

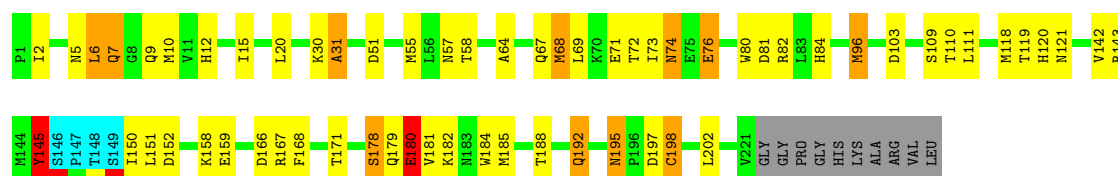
Chain B: 71% 19% . . .



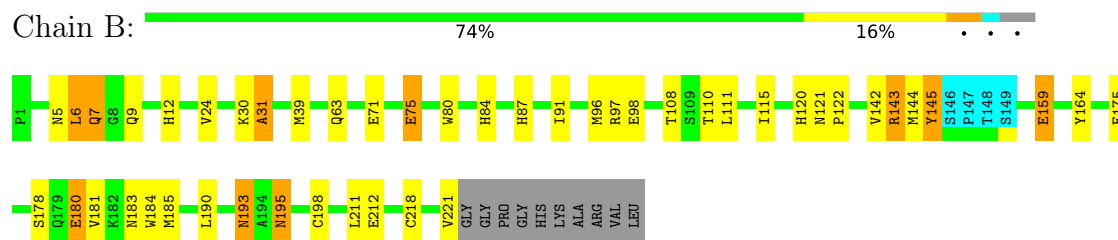
4.2.79 Score per residue for model 79

• Molecule 1: Capsid protein p24

Chain A: 67% 21% 5% . . .

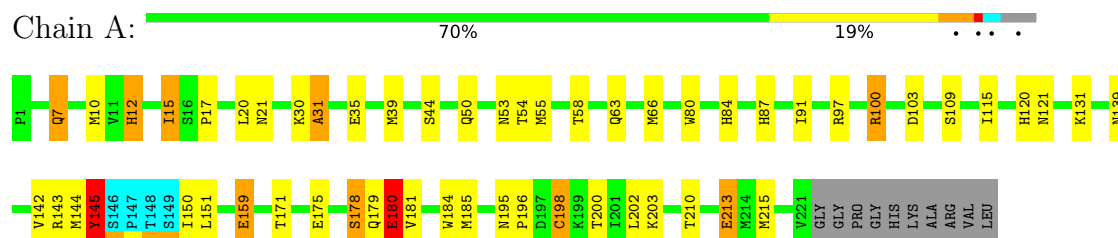


• Molecule 1: Capsid protein p24

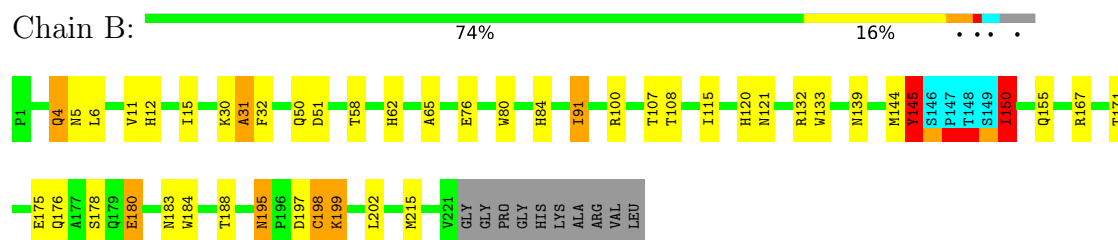


4.2.80 Score per residue for model 80

- Molecule 1: Capsid protein p24

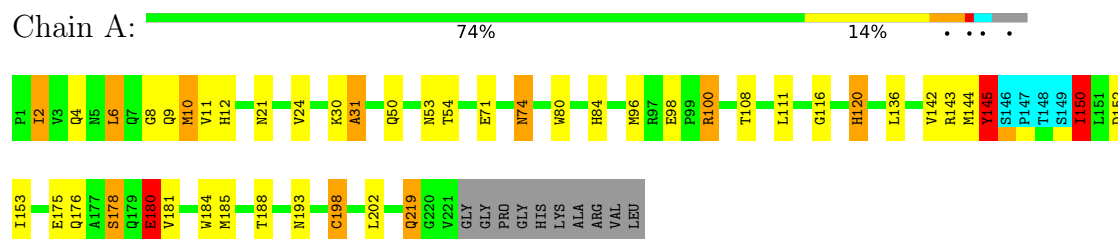


- Molecule 1: Capsid protein p24

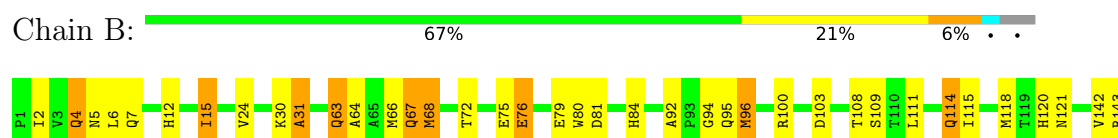


4.2.81 Score per residue for model 81

- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24





4.2.82 Score per residue for model 82

- Molecule 1: Capsid protein p24

Chain A: 68% 22% . . .



- Molecule 1: Capsid protein p24

Chain B: 72% 19% . . .



4.2.83 Score per residue for model 83

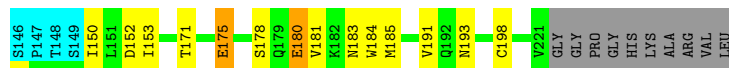
- Molecule 1: Capsid protein p24

Chain A: 74% 15% . . .



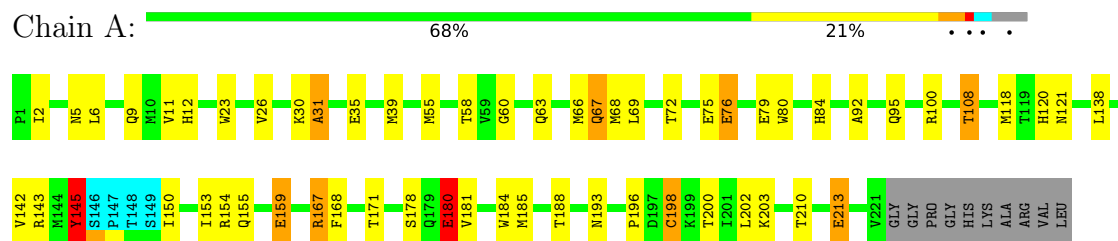
- Molecule 1: Capsid protein p24

Chain B: 73% 19% . . .

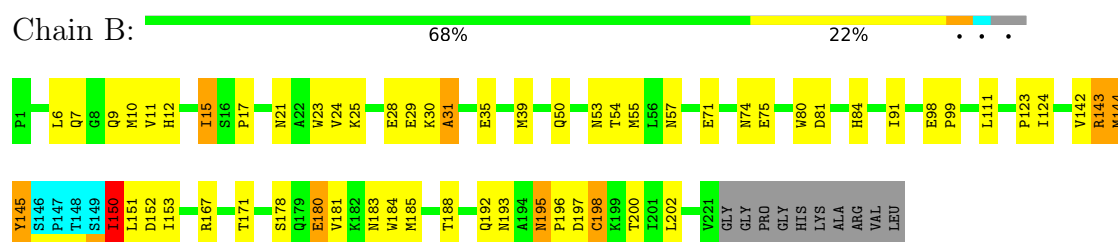


4.2.84 Score per residue for model 84

- Molecule 1: Capsid protein p24

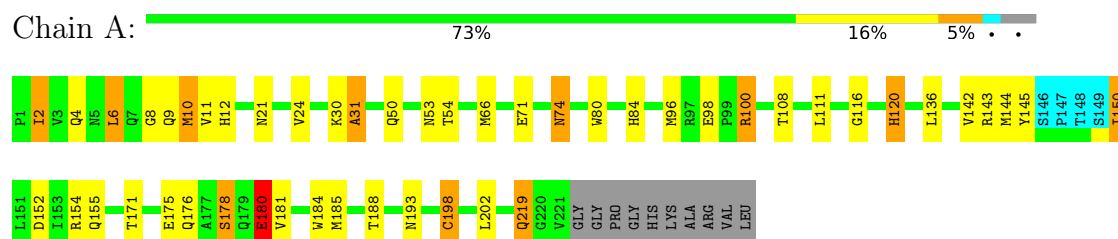


- Molecule 1: Capsid protein p24

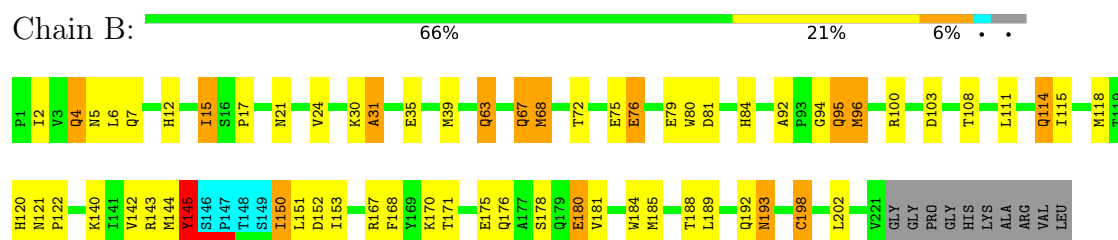


4.2.85 Score per residue for model 85

- Molecule 1: Capsid protein p24

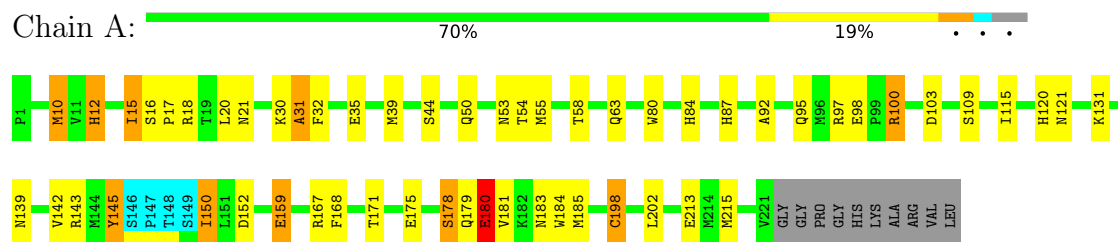


- Molecule 1: Capsid protein p24

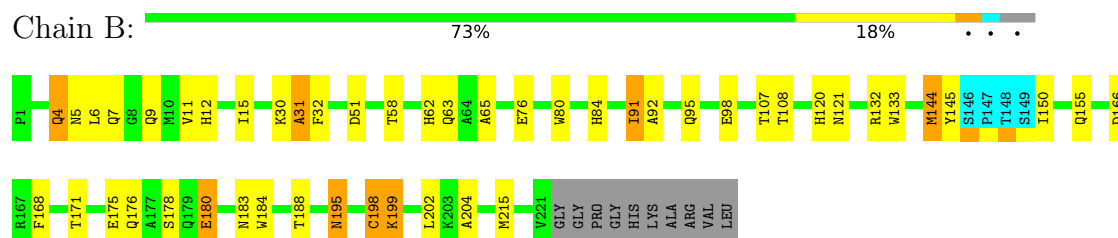


4.2.86 Score per residue for model 86

- Molecule 1: Capsid protein p24

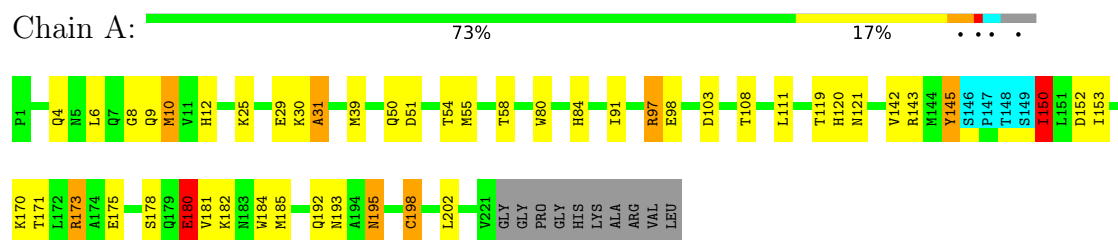


- Molecule 1: Capsid protein p24

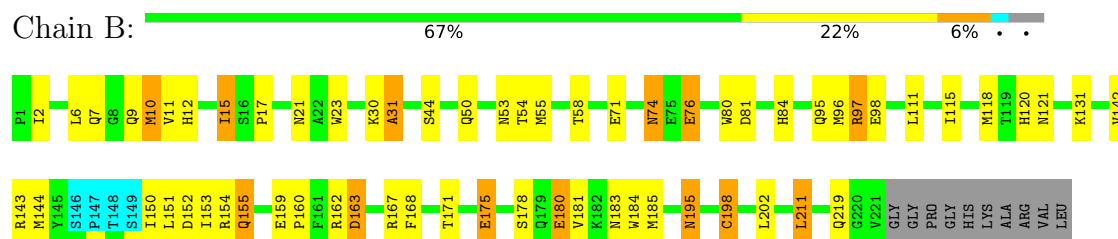


4.2.87 Score per residue for model 87

- Molecule 1: Capsid protein p24

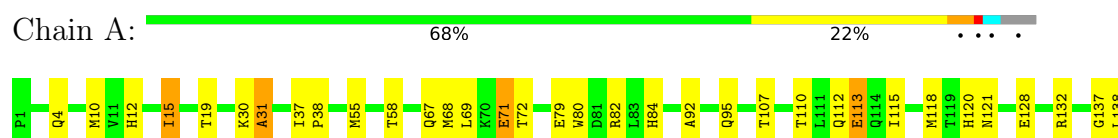


- Molecule 1: Capsid protein p24



4.2.88 Score per residue for model 88

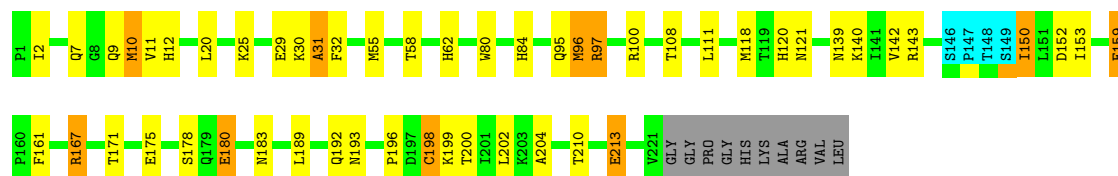
- Molecule 1: Capsid protein p24





• Molecule 1: Capsid protein p24

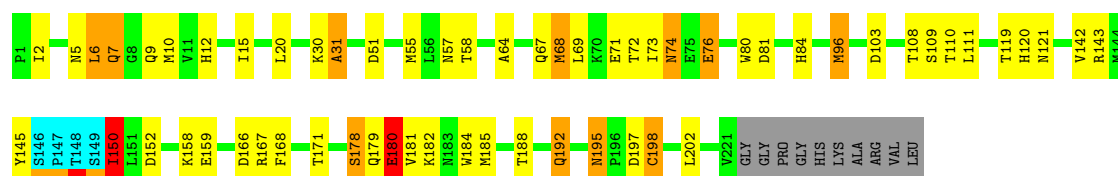
Chain B: 71% 18% . . .



4.2.89 Score per residue for model 89

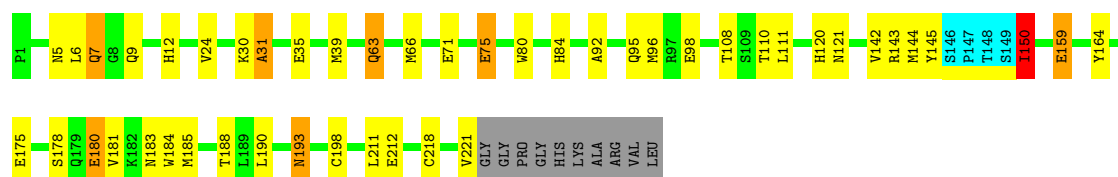
• Molecule 1: Capsid protein p24

Chain A: 68% 20% 5% . . .



• Molecule 1: Capsid protein p24

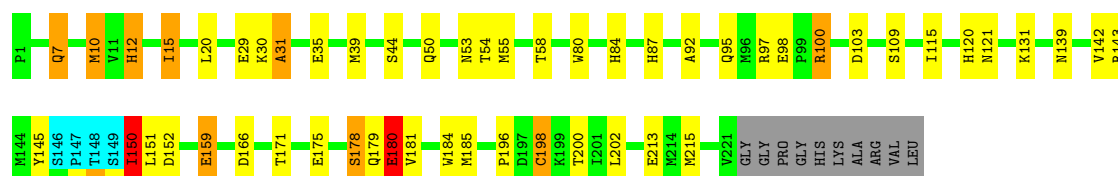
Chain B: 74% 17% . . .



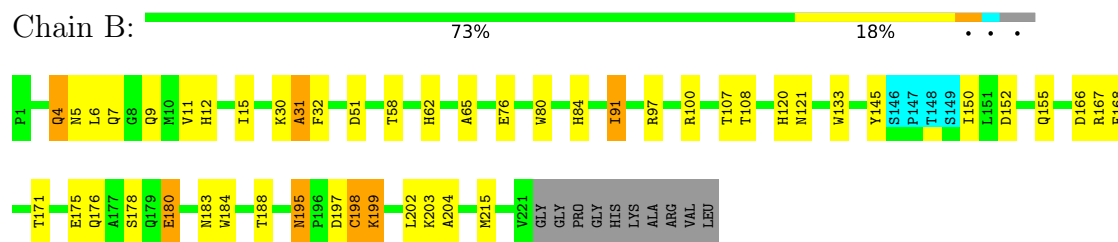
4.2.90 Score per residue for model 90

• Molecule 1: Capsid protein p24

Chain A: 71% 18% . . .

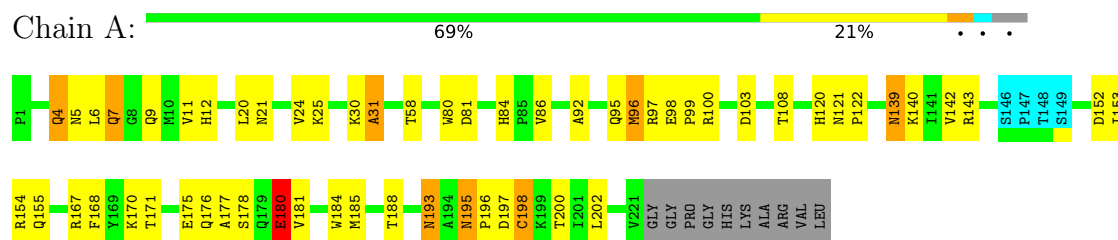


• Molecule 1: Capsid protein p24

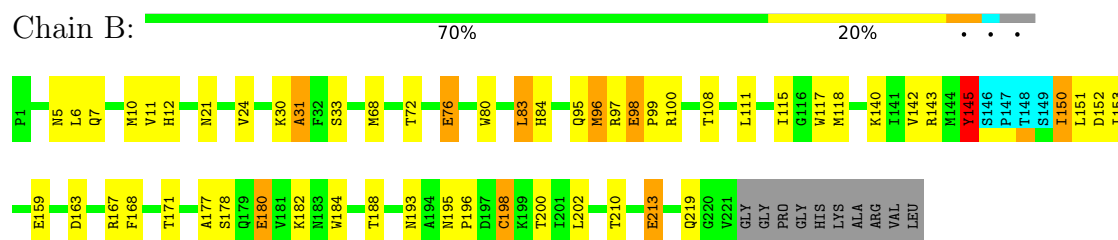


4.2.91 Score per residue for model 91

- Molecule 1: Capsid protein p24

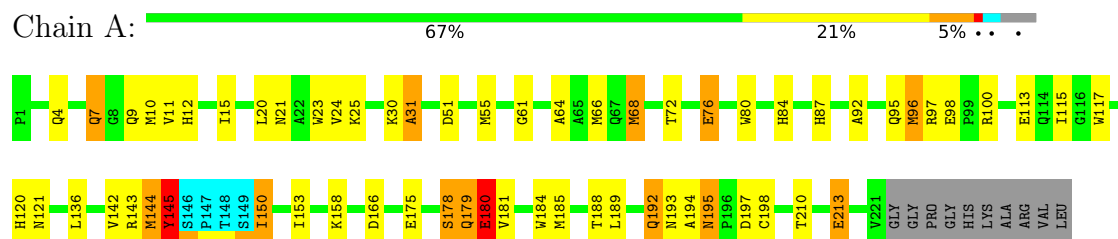


- Molecule 1: Capsid protein p24

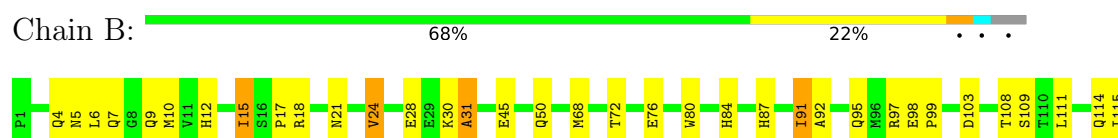


4.2.92 Score per residue for model 92

- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24



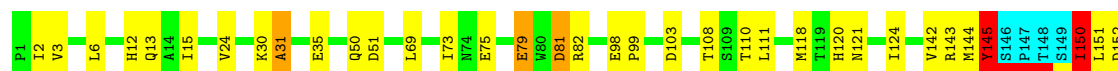


4.2.93 Score per residue for model 93

- Molecule 1: Capsid protein p24

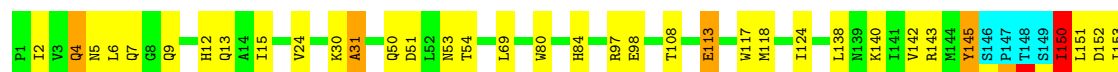


- Molecule 1: Capsid protein p24

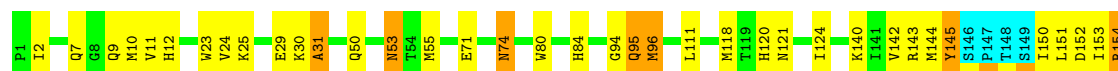


4.2.94 Score per residue for model 94

- Molecule 1: Capsid protein p24

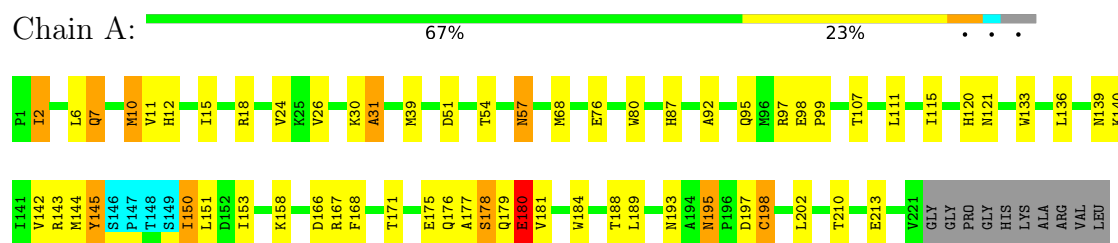


- Molecule 1: Capsid protein p24

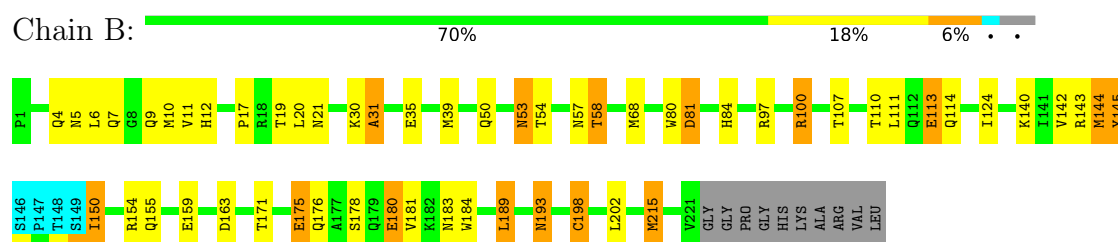


4.2.97 Score per residue for model 97

- Molecule 1: Capsid protein p24

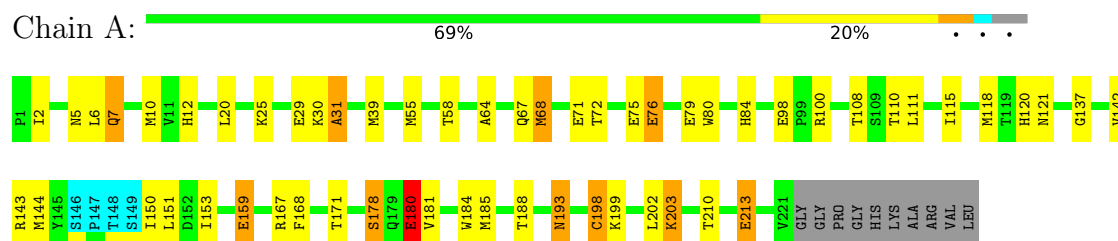


- Molecule 1: Capsid protein p24

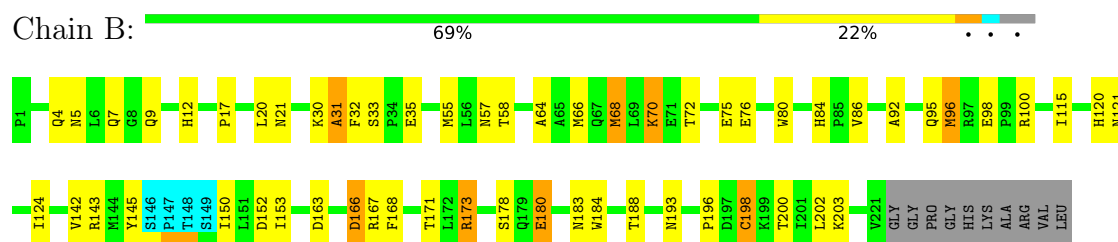


4.2.98 Score per residue for model 98

- Molecule 1: Capsid protein p24

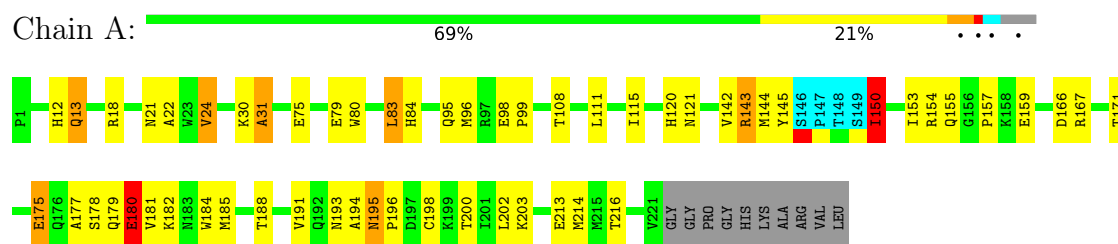


- Molecule 1: Capsid protein p24

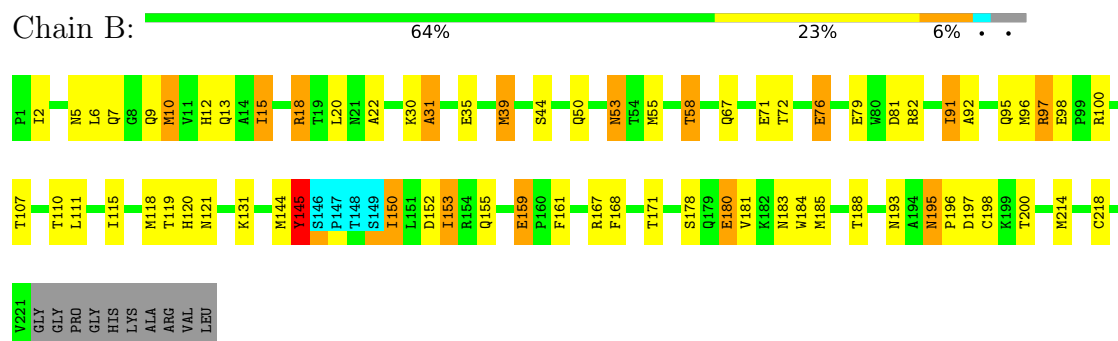


4.2.99 Score per residue for model 99

- Molecule 1: Capsid protein p24

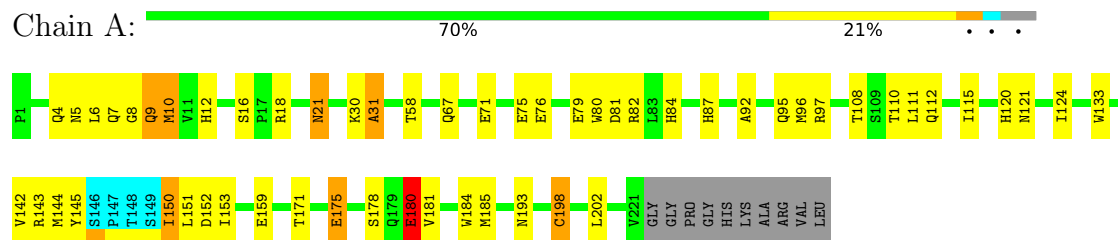


- Molecule 1: Capsid protein p24

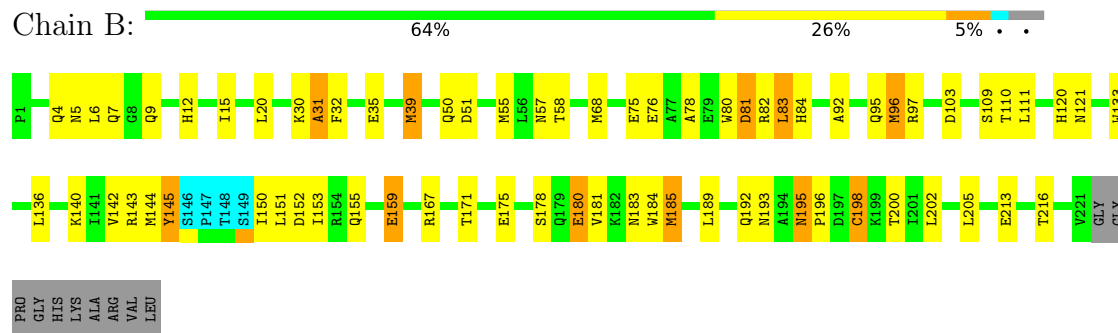


4.2.100 Score per residue for model 100

- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24



5 Refinement protocol and experimental data overview

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

Of the 480 calculated structures, 100 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	2.32

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	919
Number of shifts mapped to atoms	875
Number of unparsed shifts	0
Number of shifts with mapping errors	44
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	15%

6 Model quality i

6.1 Standard geometry i

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	0.56±0.04	1±1/1737 (0.1± 0.1%)	0.87±0.01	2±1/2360 (0.1± 0.0%)
1	B	0.55±0.03	1±1/1737 (0.0± 0.0%)	0.85±0.02	1±1/2360 (0.0± 0.0%)
All	All	0.56	148/347400 (0.0%)	0.86	256/472000 (0.1%)

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	0.0±0.1
All	All	0	1

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	145	TYR	N-CA	18.47	1.70	1.46	97	23
1	A	145	TYR	CA-C	15.30	1.73	1.52	92	22
1	B	145	TYR	CA-C	13.48	1.68	1.52	91	20
1	A	145	TYR	N-CA	12.01	1.61	1.46	84	34
1	B	150	ILE	CA-C	10.11	1.65	1.52	80	6
1	A	150	ILE	N-CA	9.18	1.57	1.46	76	8
1	A	150	ILE	CA-C	9.05	1.64	1.52	59	12
1	A	145	TYR	C-N	8.38	1.44	1.33	4	9
1	B	145	TYR	C-N	8.37	1.45	1.33	91	5
1	B	150	ILE	N-CA	6.88	1.54	1.46	80	5
1	A	145	TYR	CA-CB	5.59	1.61	1.53	87	1
1	A	150	ILE	C-N	-5.54	1.26	1.34	16	2
1	A	150	ILE	CA-CB	5.20	1.61	1.54	16	1

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	B	144	MET	CA-C-N	-13.33	102.37	122.09	97	13
1	B	144	MET	C-N-CA	-13.33	102.37	122.09	97	13
1	B	145	TYR	N-CA-C	11.89	129.93	109.96	97	17
1	A	150	ILE	N-CA-C	10.47	119.89	111.62	93	5
1	A	180	GLU	N-CA-CB	9.78	125.44	110.28	1	100
1	A	145	TYR	N-CA-C	9.77	125.56	109.24	23	18
1	B	145	TYR	N-CA-CB	9.35	126.29	110.49	99	8
1	A	150	ILE	CA-C-N	8.98	133.49	120.38	89	10
1	A	150	ILE	C-N-CA	8.98	133.49	120.38	89	10
1	A	144	MET	CA-C-N	-8.24	109.20	120.82	42	13
1	A	144	MET	C-N-CA	-8.24	109.20	120.82	42	13
1	B	150	ILE	N-CA-C	-8.04	104.01	113.42	15	5
1	A	145	TYR	CA-CB-CG	-7.27	100.81	113.90	81	5
1	B	150	ILE	N-CA-CB	-6.76	106.10	111.64	85	2
1	B	150	ILE	CA-C-N	6.71	129.94	120.28	43	5
1	B	150	ILE	C-N-CA	6.71	129.94	120.28	43	5
1	B	145	TYR	CA-CB-CG	-6.13	102.87	113.90	99	6
1	A	145	TYR	N-CA-CB	6.10	119.08	110.24	31	4
1	B	150	ILE	CB-CA-C	-5.71	106.86	111.71	2	2
1	A	145	TYR	CB-CA-C	-5.12	100.30	111.71	64	1
1	A	150	ILE	N-CA-CB	-5.10	104.58	110.55	12	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	145	TYR	Sidechain	1

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	1699	1708	1703	56±10
1	B	1699	1708	1703	56±7
All	All	339800	341600	340600	10611

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:145:TYR:N	1:B:145:TYR:CA	1.53	1.70	97	1
1:A:179:GLN:HG3	1:A:180:GLU:OE2	1.29	1.26	59	24
1:A:179:GLN:CG	1:A:180:GLU:OE2	1.13	1.95	97	24
1:A:179:GLN:HG3	1:A:180:GLU:CD	1.04	1.74	97	24
1:B:6:LEU:HD22	1:B:6:LEU:H	1.01	1.16	25	19
1:B:144:MET:O	1:B:145:TYR:HA	0.99	1.55	97	1
1:B:144:MET:C	1:B:145:TYR:HA	0.98	1.82	97	1
1:A:6:LEU:H	1:A:6:LEU:HD22	0.97	1.19	34	22
1:B:144:MET:C	1:B:145:TYR:CA	0.97	2.37	97	1
1:B:167:ARG:O	1:B:171:THR:HG23	0.95	1.62	99	50
1:B:34:PRO:HG2	1:B:152:ASP:OD2	0.93	1.62	38	1
1:A:183:ASN:OD1	1:A:184:TRP:N	0.93	2.00	27	7
1:B:143:ARG:HH21	1:B:144:MET:HE1	0.90	1.26	81	12
1:B:180:GLU:OE1	1:B:183:ASN:ND2	0.86	2.08	64	50
1:B:12:HIS:CG	1:B:111:LEU:HD21	0.85	2.06	52	33
1:B:181:VAL:HG12	1:B:185:MET:HE3	0.85	1.47	62	53
1:A:139:ASN:OD1	1:A:143:ARG:NH1	0.84	2.09	35	5
1:B:180:GLU:OE1	1:B:183:ASN:OD1	0.84	1.96	42	29
1:A:150:ILE:HD12	1:A:150:ILE:H	0.84	1.31	85	7
1:A:181:VAL:HG12	1:A:185:MET:HE3	0.83	1.48	37	83
1:A:6:LEU:HD22	1:A:6:LEU:N	0.83	1.88	23	22
1:B:6:LEU:HD22	1:B:6:LEU:N	0.83	1.88	49	40
1:A:6:LEU:N	1:A:6:LEU:HD22	0.83	1.88	84	31
1:A:184:TRP:CD1	1:A:188:THR:HG1	0.83	1.91	49	22
1:B:144:MET:O	1:B:145:TYR:C	0.83	2.21	76	24
1:A:150:ILE:H	1:A:150:ILE:HD13	0.83	1.34	40	2
1:B:12:HIS:CD2	1:B:111:LEU:HD11	0.82	2.10	12	42
1:A:61:GLY:O	1:A:158:LYS:CE	0.82	2.27	92	1
1:A:150:ILE:HG22	1:A:151:LEU:N	0.81	1.90	76	1
1:A:194:ALA:HB1	1:A:198:CYS:SG	0.80	2.16	62	5
1:A:21:ASN:OD1	1:A:22:ALA:N	0.80	2.15	99	2
1:A:21:ASN:ND2	1:A:25:LYS:HZ3	0.79	1.75	12	2
1:B:164:TYR:OH	1:B:190:LEU:O	0.79	2.01	89	3
1:A:144:MET:O	1:A:145:TYR:C	0.79	2.24	18	24
1:A:6:LEU:HD22	1:A:6:LEU:H	0.79	1.35	60	7
1:B:68:MET:HE3	1:B:144:MET:HE1	0.78	1.56	51	4
1:A:167:ARG:O	1:A:171:THR:HG23	0.77	1.78	94	46
1:B:74:ASN:OD1	1:B:75:GLU:N	0.77	2.17	4	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:150:ILE:HG23	1:B:151:LEU:H	0.77	1.39	93	9
1:A:179:GLN:HG3	1:A:180:GLU:OE1	0.77	1.79	97	13
1:A:150:ILE:HD12	1:A:150:ILE:O	0.77	1.78	86	1
1:A:150:ILE:HD11	1:A:172:LEU:HA	0.77	1.55	78	1
1:B:34:PRO:CG	1:B:152:ASP:OD2	0.76	2.32	38	1
1:A:179:GLN:HG2	1:A:180:GLU:OE2	0.76	1.80	97	7
1:A:6:LEU:H	1:A:6:LEU:CD2	0.76	1.94	50	28
1:B:6:LEU:H	1:B:6:LEU:CD2	0.76	1.93	46	18
1:A:150:ILE:N	1:A:150:ILE:HD13	0.75	1.97	42	5
1:A:51:ASP:O	1:A:54:THR:OG1	0.74	2.04	77	3
1:A:150:ILE:HG23	1:A:151:LEU:H	0.74	1.40	88	11
1:A:150:ILE:HD12	1:A:150:ILE:N	0.74	1.98	24	6
1:B:166:ASP:OD2	1:B:167:ARG:NH2	0.73	2.21	43	3
1:B:198:CYS:HG	1:B:218:CYS:HG	0.73	1.26	49	1
1:B:144:MET:O	1:B:145:TYR:O	0.73	2.06	93	6
1:B:161:PHE:CG	1:B:218:CYS:SG	0.73	2.81	57	6
1:A:144:MET:O	1:A:145:TYR:CD1	0.73	2.41	78	2
1:A:6:LEU:HD23	1:A:6:LEU:O	0.73	1.82	66	2
1:A:98:GLU:CD	1:A:100:ARG:HH22	0.73	1.91	85	17
1:A:175:GLU:OE2	1:A:185:MET:HE1	0.73	1.84	62	3
1:A:91:ILE:HD11	1:A:97:ARG:CZ	0.73	2.14	31	4
1:A:53:ASN:OD1	1:A:54:THR:N	0.72	2.22	14	27
1:A:175:GLU:OE1	1:A:177:ALA:HB2	0.72	1.84	97	9
1:B:53:ASN:OD1	1:B:54:THR:N	0.72	2.23	75	18
1:A:12:HIS:CD2	1:A:111:LEU:HD11	0.72	2.19	69	44
1:A:81:ASP:OD1	1:A:82:ARG:N	0.72	2.23	48	10
1:B:175:GLU:OE1	1:B:177:ALA:HB2	0.72	1.85	68	1
1:A:143:ARG:NH2	1:A:170:LYS:NZ	0.71	2.38	43	1
1:B:32:PHE:CE1	1:B:62:HIS:NE2	0.71	2.58	33	9
1:B:150:ILE:HD12	1:B:150:ILE:N	0.71	2.00	57	7
1:A:157:PRO:HA	1:A:195:ASN:ND2	0.70	2.01	99	2
1:A:139:ASN:CG	1:A:167:ARG:HD3	0.70	2.11	51	1
1:A:139:ASN:CG	1:A:143:ARG:NH1	0.70	2.49	35	4
1:A:55:MET:O	1:A:58:THR:OG1	0.70	2.09	17	14
1:B:91:ILE:HD12	1:B:91:ILE:N	0.70	2.01	59	19
1:A:150:ILE:HD13	1:A:185:MET:HE2	0.70	1.63	21	1
1:A:29:GLU:OE2	1:B:203:LYS:O	0.70	2.09	90	1
1:A:97:ARG:NE	1:A:97:ARG:H	0.70	1.85	87	1
1:A:139:ASN:ND2	1:A:167:ARG:NH1	0.70	2.40	3	1
1:B:95:GLN:NE2	1:B:95:GLN:N	0.70	2.40	26	13
1:B:108:THR:HG22	1:B:108:THR:O	0.69	1.86	73	32

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:ILE:C	1:A:2:ILE:HD13	0.69	2.13	68	1
1:A:145:TYR:CG	1:A:145:TYR:O	0.69	2.46	47	1
1:B:150:ILE:HG22	1:B:151:LEU:H	0.69	1.46	64	1
1:A:32:PHE:CZ	1:A:145:TYR:CD1	0.69	2.81	72	1
1:B:167:ARG:HH21	1:B:171:THR:N	0.69	1.85	39	8
1:A:80:TRP:CE3	1:A:84:HIS:CE1	0.69	2.80	85	35
1:B:96:MET:N	1:B:96:MET:SD	0.69	2.66	34	31
1:A:100:ARG:CD	1:A:101:GLY:H	0.69	2.00	57	4
1:B:97:ARG:H	1:B:97:ARG:NE	0.69	1.86	88	5
1:B:32:PHE:CZ	1:B:145:TYR:CD2	0.68	2.81	43	1
1:A:20:LEU:C	1:A:20:LEU:HD23	0.68	2.14	82	7
1:A:41:SER:HB3	1:B:203:LYS:O	0.68	1.88	70	1
1:B:92:ALA:HB3	1:B:95:GLN:OE1	0.68	1.88	43	21
1:A:92:ALA:HB3	1:A:95:GLN:OE1	0.68	1.89	9	24
1:B:81:ASP:OD1	1:B:82:ARG:N	0.68	2.27	49	4
1:A:143:ARG:O	1:A:143:ARG:CZ	0.68	2.42	17	7
1:A:179:GLN:HE22	1:A:182:LYS:NZ	0.68	1.87	69	4
1:A:108:THR:O	1:A:108:THR:HG22	0.68	1.87	51	17
1:B:210:THR:HG1	1:B:213:GLU:CD	0.68	1.97	78	6
1:B:171:THR:O	1:B:175:GLU:OE2	0.68	2.12	78	6
1:A:97:ARG:HE	1:A:97:ARG:H	0.67	1.32	32	1
1:A:97:ARG:H	1:A:97:ARG:NE	0.67	1.87	32	1
1:B:184:TRP:CH2	1:B:189:LEU:HD23	0.67	2.25	58	13
1:B:7:GLN:O	1:B:9:GLN:OE1	0.67	2.12	89	15
1:A:66:MET:HE3	1:A:67:GLN:NE2	0.67	2.05	74	4
1:B:161:PHE:CD2	1:B:218:CYS:SG	0.67	2.87	99	2
1:B:97:ARG:HE	1:B:98:GLU:H	0.67	1.32	11	9
1:B:143:ARG:NH1	1:B:154:ARG:NE	0.67	2.43	66	1
1:A:15:ILE:HG22	1:A:19:THR:OG1	0.67	1.90	28	13
1:A:5:ASN:HD21	1:A:7:GLN:NE2	0.66	1.88	91	6
1:A:172:LEU:C	1:A:172:LEU:HD13	0.66	2.15	68	1
1:A:139:ASN:ND2	1:A:143:ARG:NH1	0.66	2.43	35	5
1:B:159:GLU:N	1:B:159:GLU:OE1	0.66	2.28	48	31
1:A:150:ILE:HG23	1:A:151:LEU:N	0.66	2.05	100	13
1:B:92:ALA:HB3	1:B:95:GLN:NE2	0.66	2.05	30	13
1:A:6:LEU:N	1:A:6:LEU:CD2	0.66	2.59	9	31
1:A:80:TRP:CZ3	1:A:84:HIS:CE1	0.66	2.84	10	58
1:A:2:ILE:HD12	1:A:2:ILE:N	0.66	2.06	37	7
1:B:150:ILE:HG23	1:B:151:LEU:N	0.66	2.06	44	13
1:B:5:ASN:HD22	1:B:9:GLN:NE2	0.66	1.89	38	9
1:A:161:PHE:CD2	1:A:218:CYS:SG	0.66	2.88	69	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:6:LEU:N	1:B:6:LEU:CD2	0.65	2.59	10	54
1:A:159:GLU:N	1:A:159:GLU:OE1	0.65	2.29	86	39
1:A:140:LYS:NZ	1:A:143:ARG:NH2	0.65	2.44	14	3
1:A:97:ARG:NH1	1:A:100:ARG:CZ	0.65	2.59	75	3
1:B:143:ARG:NH1	1:B:170:LYS:HZ3	0.65	1.88	28	1
1:B:80:TRP:CZ3	1:B:84:HIS:NE2	0.65	2.65	7	33
1:B:57:ASN:OD1	1:B:58:THR:N	0.65	2.29	52	2
1:B:80:TRP:CZ3	1:B:84:HIS:CE1	0.65	2.84	6	48
1:A:84:HIS:O	1:A:100:ARG:NH2	0.65	2.29	36	29
1:B:87:HIS:CE1	1:B:97:ARG:NH1	0.65	2.64	56	7
1:A:161:PHE:CG	1:A:218:CYS:SG	0.65	2.84	69	1
1:B:219:GLN:N	1:B:219:GLN:OE1	0.65	2.30	49	4
1:A:71:GLU:O	1:A:74:ASN:ND2	0.65	2.30	34	3
1:B:97:ARG:H	1:B:97:ARG:HE	0.65	1.35	88	2
1:A:2:ILE:H	1:A:2:ILE:HD13	0.65	1.52	1	18
1:B:142:VAL:O	1:B:145:TYR:CE1	0.65	2.50	11	1
1:A:15:ILE:HG21	1:A:55:MET:HE2	0.65	1.69	13	11
1:A:61:GLY:O	1:A:158:LYS:HE3	0.65	1.92	92	1
1:A:4:GLN:CD	1:A:5:ASN:O	0.64	2.40	15	16
1:A:5:ASN:ND2	1:A:9:GLN:NE2	0.64	2.46	9	7
1:A:180:GLU:O	1:A:183:ASN:OD1	0.64	2.15	37	7
1:B:50:GLN:O	1:B:53:ASN:OD1	0.64	2.15	87	26
1:B:154:ARG:O	1:B:167:ARG:NH2	0.64	2.31	14	6
1:A:150:ILE:HD12	1:A:185:MET:SD	0.64	2.33	78	2
1:A:30:LYS:O	1:A:31:ALA:C	0.64	2.41	27	100
1:A:21:ASN:ND2	1:A:25:LYS:NZ	0.64	2.46	92	3
1:B:30:LYS:O	1:B:31:ALA:C	0.64	2.41	11	100
1:B:155:GLN:HE22	1:B:195:ASN:ND2	0.64	1.91	87	4
1:B:81:ASP:OD2	1:B:100:ARG:NH1	0.64	2.31	81	16
1:A:143:ARG:O	1:A:143:ARG:NE	0.64	2.31	42	6
1:A:150:ILE:CG2	1:A:151:LEU:N	0.64	2.60	76	11
1:A:150:ILE:HG22	1:A:151:LEU:H	0.64	1.51	76	1
1:B:32:PHE:CE2	1:B:145:TYR:CZ	0.64	2.86	98	2
1:A:80:TRP:CZ3	1:A:84:HIS:NE2	0.64	2.66	22	16
1:A:9:GLN:NE2	1:A:9:GLN:H	0.64	1.91	89	4
1:A:97:ARG:H	1:A:97:ARG:HE	0.64	1.36	87	1
1:B:98:GLU:O	1:B:100:ARG:NH2	0.64	2.31	35	1
1:B:161:PHE:CD1	1:B:198:CYS:SG	0.64	2.91	54	3
1:B:2:ILE:HD12	1:B:2:ILE:N	0.64	2.07	69	1
1:B:144:MET:SD	1:B:154:ARG:NH1	0.64	2.71	64	1
1:B:100:ARG:NH2	1:B:102:SER:N	0.64	2.46	83	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:ILE:HD12	1:A:150:ILE:C	0.64	2.18	86	1
1:B:80:TRP:CE3	1:B:84:HIS:CE1	0.63	2.86	55	34
1:A:82:ARG:O	1:A:82:ARG:NE	0.63	2.32	82	7
1:A:139:ASN:HD21	1:A:143:ARG:NH1	0.63	1.92	80	4
1:B:32:PHE:CZ	1:B:145:TYR:CD1	0.63	2.86	8	2
1:A:143:ARG:NH2	1:A:144:MET:HE2	0.63	2.08	45	3
1:B:6:LEU:O	1:B:6:LEU:HD13	0.63	1.94	70	2
1:A:91:ILE:N	1:A:91:ILE:HD12	0.63	2.09	66	2
1:B:32:PHE:CE2	1:B:145:TYR:CE2	0.63	2.87	23	3
1:A:195:ASN:N	1:A:198:CYS:SG	0.63	2.72	54	5
1:B:120:HIS:ND1	1:B:121:ASN:N	0.63	2.47	74	19
1:B:150:ILE:CG1	1:B:151:LEU:H	0.63	2.06	22	1
1:A:87:HIS:H	1:A:97:ARG:HH22	0.63	1.35	49	4
1:B:63:GLN:NE2	1:B:64:ALA:N	0.63	2.47	28	1
1:B:184:TRP:CD1	1:B:188:THR:HG1	0.63	2.12	30	27
1:A:20:LEU:HD11	1:A:58:THR:HG21	0.63	1.71	74	4
1:A:150:ILE:HG12	1:A:151:LEU:N	0.63	2.09	94	2
1:B:56:LEU:HD23	1:B:56:LEU:O	0.63	1.94	7	7
1:A:20:LEU:HD23	1:A:55:MET:SD	0.63	2.34	31	30
1:A:184:TRP:CH2	1:B:184:TRP:CH2	0.63	2.87	3	18
1:B:175:GLU:OE1	1:B:175:GLU:N	0.62	2.32	92	6
1:B:143:ARG:NH2	1:B:144:MET:SD	0.62	2.72	29	6
1:B:17:PRO:O	1:B:21:ASN:ND2	0.62	2.33	47	13
1:A:73:ILE:HD11	1:A:134:ILE:CD1	0.62	2.24	56	8
1:B:4:GLN:CD	1:B:5:ASN:O	0.62	2.43	96	15
1:A:150:ILE:HD12	1:A:151:LEU:H	0.62	1.53	69	5
1:B:5:ASN:HD21	1:B:7:GLN:NE2	0.62	1.93	91	3
1:A:178:SER:OG	1:B:180:GLU:HG2	0.62	1.94	12	56
1:A:144:MET:O	1:A:145:TYR:O	0.62	2.18	92	3
1:B:168:PHE:O	1:B:171:THR:OG1	0.62	2.18	62	56
1:A:154:ARG:NE	1:A:155:GLN:O	0.62	2.32	44	13
1:B:150:ILE:HD12	1:B:150:ILE:H	0.62	1.54	98	5
1:B:82:ARG:O	1:B:82:ARG:NE	0.62	2.33	54	1
1:A:168:PHE:O	1:A:171:THR:OG1	0.62	2.18	21	63
1:A:5:ASN:ND2	1:A:7:GLN:NE2	0.62	2.47	18	6
1:B:142:VAL:O	1:B:145:TYR:O	0.62	2.17	48	8
1:B:97:ARG:HE	1:B:98:GLU:N	0.62	1.92	69	6
1:B:139:ASN:ND2	1:B:170:LYS:NZ	0.62	2.47	38	1
1:B:87:HIS:O	1:B:97:ARG:NH1	0.61	2.32	71	16
1:A:79:GLU:OE1	1:B:75:GLU:OE1	0.61	2.18	35	1
1:B:95:GLN:NE2	1:B:96:MET:O	0.61	2.32	11	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:ILE:HD13	1:A:118:MET:SD	0.61	2.34	48	10
1:A:16:SER:OG	1:A:18:ARG:CZ	0.61	2.48	52	1
1:A:97:ARG:NH2	1:A:100:ARG:NH2	0.61	2.48	95	5
1:A:162:ARG:NH2	1:A:219:GLN:NE2	0.61	2.47	48	2
1:B:143:ARG:HH12	1:B:167:ARG:NH2	0.61	1.94	37	1
1:B:20:LEU:HD11	1:B:58:THR:HG21	0.61	1.71	97	4
1:A:195:ASN:ND2	1:A:196:PRO:HD2	0.61	2.09	54	2
1:A:21:ASN:HD21	1:A:25:LYS:HZ1	0.61	1.38	62	1
1:A:203:LYS:O	1:B:41:SER:OG	0.61	2.12	70	1
1:A:180:GLU:CB	1:B:180:GLU:HB2	0.61	2.26	1	100
1:A:97:ARG:HH21	1:A:100:ARG:NH2	0.61	1.94	12	8
1:A:96:MET:SD	1:A:120:HIS:CE1	0.61	2.94	26	17
1:A:95:GLN:NE2	1:A:96:MET:O	0.61	2.34	37	7
1:A:7:GLN:O	1:A:9:GLN:OE1	0.61	2.19	89	12
1:A:50:GLN:O	1:A:54:THR:HG23	0.61	1.96	87	3
1:A:11:VAL:HG22	1:A:12:HIS:N	0.61	2.11	6	29
1:A:152:ASP:CG	1:A:152:ASP:O	0.61	2.44	15	53
1:A:84:HIS:O	1:A:100:ARG:NH1	0.61	2.34	37	12
1:B:145:TYR:CD1	1:B:145:TYR:C	0.61	2.79	85	6
1:A:80:TRP:CE3	1:A:84:HIS:CD2	0.61	2.89	22	10
1:B:12:HIS:NE2	1:B:48:THR:HG21	0.61	2.11	22	4
1:B:97:ARG:HE	1:B:97:ARG:H	0.61	1.38	33	1
1:B:139:ASN:HD22	1:B:170:LYS:CE	0.61	2.08	43	2
1:B:166:ASP:CG	1:B:167:ARG:N	0.61	2.59	98	2
1:A:116:GLY:O	1:A:120:HIS:ND1	0.61	2.34	10	13
1:A:167:ARG:HH21	1:A:171:THR:N	0.60	1.93	31	3
1:B:63:GLN:OE1	1:B:63:GLN:N	0.60	2.33	85	3
1:A:10:MET:SD	1:A:10:MET:N	0.60	2.74	30	33
1:A:21:ASN:HD21	1:A:25:LYS:NZ	0.60	1.94	12	3
1:B:63:GLN:CD	1:B:64:ALA:N	0.60	2.59	1	13
1:B:68:MET:SD	1:B:68:MET:N	0.60	2.74	66	5
1:B:132:ARG:NH2	1:B:133:TRP:HE1	0.60	1.95	70	3
1:B:142:VAL:O	1:B:145:TYR:CD1	0.60	2.54	11	1
1:A:181:VAL:O	1:A:185:MET:SD	0.60	2.59	34	8
1:A:21:ASN:HD21	1:A:25:LYS:HZ3	0.60	1.38	92	1
1:B:120:HIS:CG	1:B:121:ASN:N	0.60	2.70	85	79
1:A:175:GLU:OE1	1:A:176:GLN:C	0.60	2.44	67	15
1:A:96:MET:SD	1:A:96:MET:N	0.60	2.75	65	20
1:B:68:MET:SD	1:B:140:LYS:NZ	0.60	2.75	11	16
1:A:154:ARG:O	1:A:167:ARG:NH2	0.60	2.35	73	8
1:B:161:PHE:CD1	1:B:218:CYS:SG	0.60	2.94	22	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:6:LEU:CD2	1:B:6:LEU:H	0.60	2.10	41	7
1:A:97:ARG:NH1	1:A:100:ARG:NH1	0.60	2.50	50	3
1:A:159:GLU:OE1	1:A:167:ARG:NH2	0.60	2.35	89	2
1:A:180:GLU:N	1:A:180:GLU:CD	0.60	2.59	1	77
1:A:180:GLU:CD	1:A:180:GLU:N	0.60	2.59	2	23
1:A:196:PRO:O	1:A:200:THR:HG23	0.60	1.97	66	29
1:B:12:HIS:CG	1:B:111:LEU:HD11	0.60	2.31	62	21
1:A:18:ARG:HH21	1:A:22:ALA:CA	0.60	2.09	93	3
1:B:12:HIS:CE1	1:B:50:GLN:HE22	0.60	2.15	21	10
1:A:143:ARG:HH22	1:A:144:MET:HE2	0.60	1.57	45	2
1:B:80:TRP:CE3	1:B:84:HIS:CD2	0.60	2.90	53	24
1:B:96:MET:SD	1:B:117:TRP:NE1	0.60	2.75	11	6
1:B:96:MET:SD	1:B:120:HIS:NE2	0.60	2.75	64	13
1:B:195:ASN:N	1:B:198:CYS:SG	0.60	2.75	22	4
1:A:132:ARG:NH1	1:B:204:ALA:O	0.60	2.35	88	1
1:B:5:ASN:ND2	1:B:7:GLN:HE21	0.60	1.95	96	2
1:B:86:VAL:N	1:B:100:ARG:HH12	0.59	1.95	72	9
1:B:76:GLU:OE1	1:B:133:TRP:CE2	0.59	2.55	47	17
1:B:139:ASN:ND2	1:B:143:ARG:HE	0.59	1.95	92	2
1:A:119:THR:O	1:A:119:THR:HG22	0.59	1.97	89	3
1:B:143:ARG:CZ	1:B:154:ARG:NH2	0.59	2.65	60	1
1:B:5:ASN:HD21	1:B:7:GLN:HE21	0.59	1.38	96	2
1:A:4:GLN:NE2	1:A:8:GLY:O	0.59	2.35	41	20
1:B:184:TRP:CD1	1:B:188:THR:OG1	0.59	2.55	21	61
1:B:50:GLN:OE1	1:B:111:LEU:HD13	0.59	1.97	12	6
1:A:153:ILE:O	1:A:153:ILE:CG2	0.59	2.50	78	6
1:A:68:MET:N	1:A:68:MET:SD	0.59	2.75	49	10
1:B:11:VAL:HG22	1:B:12:HIS:N	0.59	2.13	33	7
1:B:114:GLN:N	1:B:114:GLN:OE1	0.59	2.35	36	14
1:A:12:HIS:CE1	1:A:50:GLN:NE2	0.59	2.70	7	7
1:B:143:ARG:NH2	1:B:144:MET:HE1	0.59	2.09	45	7
1:B:32:PHE:CZ	1:B:62:HIS:NE2	0.59	2.71	78	2
1:A:161:PHE:CD1	1:A:198:CYS:SG	0.59	2.95	69	1
1:B:5:ASN:ND2	1:B:7:GLN:NE2	0.59	2.51	100	3
1:B:50:GLN:O	1:B:53:ASN:ND2	0.59	2.36	3	9
1:B:5:ASN:OD1	1:B:6:LEU:N	0.59	2.36	62	15
1:B:66:MET:SD	1:B:70:LYS:NZ	0.59	2.76	98	2
1:B:163:ASP:O	1:B:166:ASP:OD2	0.59	2.19	53	2
1:A:155:GLN:O	1:A:195:ASN:OD1	0.59	2.21	99	2
1:A:184:TRP:CD1	1:A:188:THR:OG1	0.59	2.56	59	60
1:A:4:GLN:O	1:A:4:GLN:NE2	0.59	2.36	11	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:15:ILE:HG21	1:B:55:MET:HE2	0.59	1.73	62	5
1:A:16:SER:OG	1:A:18:ARG:NH2	0.59	2.36	53	1
1:A:87:HIS:O	1:A:97:ARG:NH1	0.59	2.36	13	22
1:B:181:VAL:O	1:B:185:MET:SD	0.59	2.61	100	25
1:B:164:TYR:CE1	1:B:193:ASN:OD1	0.59	2.55	34	3
1:A:153:ILE:O	1:A:193:ASN:ND2	0.59	2.36	44	32
1:A:15:ILE:H	1:A:15:ILE:HD13	0.59	1.58	80	6
1:A:145:TYR:CD2	1:A:145:TYR:O	0.59	2.55	80	3
1:A:203:LYS:NZ	1:B:30:LYS:NZ	0.59	2.50	84	1
1:A:5:ASN:OD1	1:A:6:LEU:N	0.59	2.36	23	35
1:A:95:GLN:OE1	1:A:95:GLN:N	0.59	2.36	73	20
1:B:35:GLU:OE2	1:B:39:MET:HE2	0.59	1.98	39	4
1:B:150:ILE:CG2	1:B:151:LEU:H	0.59	2.11	29	6
1:B:15:ILE:HD13	1:B:15:ILE:H	0.59	1.58	54	5
1:A:18:ARG:HH21	1:A:22:ALA:N	0.59	1.96	13	3
1:B:211:LEU:HD12	1:B:212:GLU:N	0.59	2.13	34	3
1:B:11:VAL:HG12	1:B:12:HIS:N	0.58	2.13	39	27
1:A:140:LYS:NZ	1:A:144:MET:SD	0.58	2.76	78	3
1:B:150:ILE:HG13	1:B:151:LEU:H	0.58	1.57	35	1
1:A:11:VAL:HG12	1:A:12:HIS:N	0.58	2.14	27	28
1:A:13:GLN:N	1:A:13:GLN:NE2	0.58	2.50	14	3
1:A:63:GLN:O	1:A:67:GLN:NE2	0.58	2.36	57	4
1:A:18:ARG:O	1:A:21:ASN:ND2	0.58	2.36	96	4
1:A:214:MET:O	1:A:218:CYS:SG	0.58	2.62	69	1
1:A:68:MET:SD	1:A:140:LYS:NZ	0.58	2.76	52	8
1:B:20:LEU:HD23	1:B:55:MET:SD	0.58	2.38	82	28
1:B:7:GLN:OE1	1:B:7:GLN:N	0.58	2.37	44	9
1:B:4:GLN:CD	1:B:4:GLN:O	0.58	2.47	90	14
1:B:7:GLN:O	1:B:7:GLN:NE2	0.58	2.36	67	5
1:B:7:GLN:O	1:B:9:GLN:NE2	0.58	2.36	9	35
1:A:4:GLN:NE2	1:A:5:ASN:O	0.58	2.37	43	10
1:A:184:TRP:NE1	1:A:188:THR:OG1	0.58	2.36	49	9
1:A:38:PRO:HB3	1:B:207:PRO:HG3	0.58	1.75	33	1
1:B:4:GLN:NE2	1:B:5:ASN:O	0.58	2.37	68	15
1:B:95:GLN:OE1	1:B:95:GLN:N	0.58	2.36	8	15
1:B:2:ILE:HD13	1:B:118:MET:SD	0.58	2.39	46	25
1:B:143:ARG:NH1	1:B:152:ASP:OD1	0.58	2.36	100	1
1:A:96:MET:SD	1:A:120:HIS:NE2	0.58	2.77	38	22
1:A:60:GLY:O	1:A:63:GLN:NE2	0.58	2.36	39	7
1:B:80:TRP:CH2	1:B:84:HIS:NE2	0.58	2.72	29	25
1:A:18:ARG:CZ	1:A:21:ASN:HD22	0.58	2.12	13	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:ILE:CG1	1:A:151:LEU:H	0.58	2.12	16	1
1:A:100:ARG:CG	1:A:101:GLY:N	0.58	2.67	57	4
1:A:9:GLN:OE1	1:A:9:GLN:N	0.58	2.36	72	19
1:A:81:ASP:CG	1:A:100:ARG:NH1	0.58	2.61	83	2
1:B:153:ILE:O	1:B:193:ASN:ND2	0.58	2.37	29	55
1:B:10:MET:SD	1:B:10:MET:N	0.58	2.76	67	20
1:A:143:ARG:NH2	1:A:170:LYS:HZ2	0.58	1.97	43	1
1:A:5:ASN:HD22	1:A:7:GLN:NE2	0.58	1.97	53	2
1:A:195:ASN:ND2	1:A:197:ASP:OD1	0.58	2.37	70	2
1:B:97:ARG:HH12	1:B:100:ARG:NE	0.58	1.97	97	1
1:A:180:GLU:HB2	1:B:180:GLU:HB2	0.58	1.74	1	100
1:B:152:ASP:O	1:B:152:ASP:OD1	0.58	2.22	93	7
1:A:139:ASN:OD1	1:A:140:LYS:N	0.58	2.36	15	6
1:A:98:GLU:OE2	1:A:100:ARG:NH1	0.58	2.37	74	12
1:B:218:CYS:O	1:B:221:VAL:HG23	0.58	1.98	34	3
1:B:177:ALA:O	1:B:182:LYS:NZ	0.58	2.37	11	17
1:A:81:ASP:OD1	1:A:81:ASP:C	0.58	2.46	73	10
1:B:7:GLN:NE2	1:B:9:GLN:CD	0.58	2.62	49	4
1:A:18:ARG:O	1:A:21:ASN:OD1	0.58	2.22	54	2
1:B:84:HIS:O	1:B:100:ARG:NH2	0.57	2.37	24	17
1:A:184:TRP:CH2	1:A:189:LEU:HD23	0.57	2.34	68	4
1:B:152:ASP:CG	1:B:152:ASP:O	0.57	2.47	3	34
1:A:91:ILE:HD11	1:A:97:ARG:NH2	0.57	2.14	80	1
1:A:54:THR:O	1:A:58:THR:HG23	0.57	1.99	57	14
1:B:179:GLN:H	1:B:179:GLN:CD	0.57	2.05	82	7
1:B:167:ARG:NH2	1:B:171:THR:OG1	0.57	2.37	39	7
1:B:161:PHE:CE1	1:B:198:CYS:SG	0.57	2.96	54	7
1:B:12:HIS:NE2	1:B:50:GLN:NE2	0.57	2.53	75	7
1:A:155:GLN:N	1:A:164:TYR:CE1	0.57	2.72	31	4
1:A:167:ARG:NH1	1:A:171:THR:HG23	0.57	2.14	84	7
1:B:9:GLN:CD	1:B:9:GLN:N	0.57	2.62	34	8
1:A:97:ARG:HE	1:A:100:ARG:NH2	0.57	1.98	12	3
1:A:21:ASN:ND2	1:A:25:LYS:HZ1	0.57	1.98	62	1
1:A:143:ARG:NH2	1:B:192:GLN:OE1	0.57	2.38	35	1
1:B:139:ASN:ND2	1:B:170:LYS:CE	0.57	2.68	38	2
1:A:79:GLU:CD	1:A:82:ARG:NH1	0.57	2.62	55	4
1:A:15:ILE:HD12	1:A:15:ILE:H	0.57	1.60	68	18
1:A:87:HIS:H	1:A:97:ARG:NH2	0.57	1.96	24	2
1:B:143:ARG:HH12	1:B:167:ARG:HH21	0.57	1.43	37	1
1:B:15:ILE:H	1:B:15:ILE:HD12	0.57	1.60	20	24
1:B:72:THR:HG21	1:B:137:GLY:HA2	0.57	1.77	67	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:23:TRP:CD1	1:B:55:MET:SD	0.57	2.98	64	11
1:A:195:ASN:OD1	1:A:197:ASP:OD1	0.57	2.22	74	7
1:A:72:THR:HG21	1:A:137:GLY:HA2	0.57	1.77	33	5
1:A:9:GLN:N	1:A:9:GLN:CD	0.57	2.63	69	4
1:A:120:HIS:CG	1:A:121:ASN:N	0.57	2.73	91	75
1:A:139:ASN:OD1	1:A:139:ASN:C	0.57	2.48	11	6
1:B:98:GLU:N	1:B:98:GLU:OE1	0.57	2.38	68	8
1:B:139:ASN:ND2	1:B:170:LYS:HE3	0.57	2.15	43	1
1:B:35:GLU:O	1:B:39:MET:SD	0.56	2.63	82	19
1:B:124:ILE:N	1:B:124:ILE:HD12	0.56	2.15	9	43
1:A:167:ARG:NH1	1:A:171:THR:CG2	0.56	2.68	39	7
1:A:96:MET:SD	1:A:97:ARG:N	0.56	2.78	46	12
1:B:214:MET:O	1:B:218:CYS:SG	0.56	2.63	47	6
1:B:96:MET:HE2	1:B:120:HIS:CE1	0.56	2.35	89	2
1:B:143:ARG:O	1:B:143:ARG:NE	0.56	2.39	42	8
1:A:5:ASN:ND2	1:A:9:GLN:CD	0.56	2.64	39	7
1:B:71:GLU:O	1:B:74:ASN:OD1	0.56	2.23	84	13
1:B:32:PHE:CE1	1:B:145:TYR:CD1	0.56	2.93	18	2
1:B:139:ASN:HD21	1:B:143:ARG:HE	0.56	1.43	12	2
1:A:17:PRO:O	1:A:21:ASN:ND2	0.56	2.37	35	5
1:B:98:GLU:O	1:B:100:ARG:NH1	0.56	2.37	34	3
1:B:164:TYR:OH	1:B:193:ASN:ND2	0.56	2.38	34	3
1:A:76:GLU:OE1	1:A:133:TRP:CE2	0.56	2.58	2	19
1:B:12:HIS:HB2	1:B:115:ILE:HD11	0.56	1.78	95	25
1:B:153:ILE:O	1:B:153:ILE:CG2	0.56	2.52	33	11
1:A:98:GLU:H	1:A:98:GLU:CD	0.56	2.08	77	15
1:A:162:ARG:NH2	1:A:219:GLN:HE22	0.56	1.99	23	2
1:B:143:ARG:NH1	1:B:170:LYS:NZ	0.56	2.52	28	1
1:A:145:TYR:O	1:A:145:TYR:CG	0.56	2.59	83	3
1:A:139:ASN:ND2	1:A:167:ARG:NE	0.56	2.52	38	1
1:A:83:LEU:O	1:A:83:LEU:HD23	0.56	2.00	54	2
1:B:153:ILE:N	1:B:153:ILE:CD1	0.56	2.68	99	2
1:B:143:ARG:HH12	1:B:154:ARG:NE	0.56	1.98	66	1
1:A:81:ASP:OD1	1:A:100:ARG:NH1	0.56	2.38	69	1
1:A:184:TRP:CZ3	1:B:184:TRP:CZ3	0.56	2.93	82	14
1:A:98:GLU:O	1:A:100:ARG:NH1	0.56	2.39	53	10
1:A:150:ILE:HD13	1:A:185:MET:SD	0.56	2.40	31	3
1:A:153:ILE:HG23	1:A:153:ILE:O	0.56	2.00	32	5
1:A:197:ASP:OD1	1:A:198:CYS:N	0.56	2.39	70	2
1:B:100:ARG:NH2	1:B:102:SER:H	0.56	1.98	83	2
1:B:153:ILE:O	1:B:153:ILE:HG23	0.56	2.00	28	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:140:LYS:O	1:B:144:MET:SD	0.56	2.63	85	5
1:B:143:ARG:O	1:B:143:ARG:CZ	0.56	2.53	42	5
1:B:87:HIS:O	1:B:97:ARG:NH2	0.56	2.38	74	6
1:B:69:LEU:O	1:B:73:ILE:HD13	0.56	2.01	13	3
1:A:78:ALA:O	1:A:81:ASP:OD1	0.56	2.24	58	10
1:A:95:GLN:O	1:A:96:MET:SD	0.56	2.64	37	10
1:A:150:ILE:N	1:A:150:ILE:CD1	0.56	2.68	42	7
1:A:140:LYS:HZ2	1:A:143:ARG:NH2	0.56	1.98	14	2
1:B:20:LEU:HD11	1:B:58:THR:OG1	0.56	2.01	48	15
1:B:97:ARG:HE	1:B:100:ARG:HH12	0.56	1.43	90	1
1:B:97:ARG:NH1	1:B:100:ARG:NE	0.56	2.54	97	1
1:A:4:GLN:OE1	1:A:10:MET:N	0.56	2.39	55	15
1:A:7:GLN:O	1:A:9:GLN:NE2	0.56	2.39	68	19
1:A:12:HIS:HB2	1:A:115:ILE:HD11	0.56	1.78	62	7
1:B:96:MET:SD	1:B:96:MET:N	0.56	2.78	51	9
1:A:96:MET:SD	1:A:97:ARG:O	0.56	2.64	75	7
1:A:69:LEU:O	1:A:73:ILE:HD13	0.56	2.01	89	7
1:A:150:ILE:CG2	1:A:151:LEU:H	0.56	2.14	25	3
1:A:192:GLN:O	1:A:199:LYS:NZ	0.56	2.39	82	8
1:B:9:GLN:H	1:B:9:GLN:NE2	0.56	1.99	34	5
1:B:98:GLU:OE2	1:B:100:ARG:NE	0.56	2.37	15	2
1:B:195:ASN:OD1	1:B:197:ASP:OD1	0.56	2.23	74	4
1:A:6:LEU:CD2	1:A:6:LEU:H	0.56	2.13	29	5
1:B:5:ASN:HD22	1:B:9:GLN:HE21	0.56	1.43	99	4
1:B:166:ASP:OD1	1:B:167:ARG:N	0.56	2.39	53	2
1:B:30:LYS:NZ	1:B:35:GLU:OE1	0.56	2.39	93	1
1:B:6:LEU:N	1:B:6:LEU:HD22	0.55	2.14	40	22
1:B:154:ARG:NH1	1:B:155:GLN:O	0.55	2.40	32	3
1:B:167:ARG:NH1	1:B:171:THR:OG1	0.55	2.39	33	3
1:A:145:TYR:CD1	1:A:145:TYR:O	0.55	2.60	52	3
1:A:7:GLN:NE2	1:A:7:GLN:N	0.55	2.54	52	2
1:A:97:ARG:NH2	1:A:113:GLU:OE2	0.55	2.40	2	4
1:A:64:ALA:O	1:A:68:MET:SD	0.55	2.65	49	12
1:B:5:ASN:ND2	1:B:6:LEU:H	0.55	1.99	76	6
1:A:7:GLN:HB3	1:A:9:GLN:HE22	0.55	1.61	89	3
1:A:192:GLN:NE2	1:A:193:ASN:ND2	0.55	2.53	66	2
1:B:143:ARG:NH2	1:B:152:ASP:OD2	0.55	2.38	70	1
1:A:198:CYS:SG	1:A:202:LEU:HD11	0.55	2.41	42	93
1:A:87:HIS:O	1:A:97:ARG:NH2	0.55	2.39	100	10
1:B:5:ASN:ND2	1:B:7:GLN:CD	0.55	2.65	15	3
1:B:164:TYR:CZ	1:B:193:ASN:OD1	0.55	2.59	34	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ARG:HE	1:A:18:ARG:H	0.55	1.44	53	1
1:A:159:GLU:OE2	1:A:167:ARG:NH2	0.55	2.40	37	3
1:B:153:ILE:CG2	1:B:153:ILE:O	0.55	2.53	13	2
1:A:7:GLN:NE2	1:A:9:GLN:CD	0.55	2.65	22	4
1:B:7:GLN:O	1:B:7:GLN:CD	0.55	2.50	58	4
1:A:167:ARG:NH2	1:A:171:THR:OG1	0.55	2.40	31	1
1:B:100:ARG:NH2	1:B:102:SER:OG	0.55	2.39	50	1
1:A:35:GLU:O	1:A:39:MET:SD	0.55	2.64	37	35
1:B:150:ILE:HD13	1:B:175:GLU:OE2	0.55	2.02	4	1
1:A:97:ARG:NH2	1:A:98:GLU:OE1	0.55	2.40	64	3
1:A:143:ARG:HH22	1:A:170:LYS:NZ	0.55	1.99	43	1
1:B:97:ARG:H	1:B:97:ARG:CD	0.55	2.15	54	2
1:A:41:SER:C	1:B:204:ALA:HA	0.55	2.27	70	1
1:A:53:ASN:OD1	1:A:53:ASN:C	0.55	2.50	26	27
1:B:44:SER:O	1:B:131:LYS:NZ	0.55	2.40	42	13
1:A:150:ILE:HD12	1:A:151:LEU:N	0.55	2.16	34	3
1:A:179:GLN:OE1	1:A:180:GLU:N	0.55	2.40	92	3
1:B:155:GLN:NE2	1:B:195:ASN:H	0.55	2.00	56	10
1:A:10:MET:HG3	1:A:119:THR:HG21	0.55	1.79	79	3
1:B:175:GLU:OE2	1:B:176:GLN:N	0.55	2.40	35	5
1:A:7:GLN:CG	1:A:7:GLN:O	0.55	2.55	53	2
1:B:63:GLN:N	1:B:63:GLN:CD	0.55	2.64	85	1
1:A:150:ILE:H	1:A:150:ILE:CD1	0.55	2.08	32	4
1:B:12:HIS:HB3	1:B:115:ILE:HD11	0.55	1.78	28	24
1:A:12:HIS:CG	1:A:111:LEU:HD21	0.55	2.37	47	20
1:B:53:ASN:OD1	1:B:53:ASN:C	0.55	2.50	50	18
1:B:167:ARG:HH21	1:B:171:THR:CA	0.55	2.15	39	5
1:B:195:ASN:ND2	1:B:197:ASP:OD1	0.55	2.40	93	7
1:A:7:GLN:N	1:A:7:GLN:OE1	0.55	2.39	95	6
1:A:175:GLU:N	1:A:175:GLU:OE1	0.55	2.40	55	13
1:B:97:ARG:NH2	1:B:98:GLU:OE1	0.55	2.40	73	7
1:B:195:ASN:HD21	1:B:197:ASP:CG	0.55	2.09	74	4
1:A:150:ILE:HD11	1:A:168:PHE:CD1	0.55	2.37	84	3
1:B:150:ILE:N	1:B:150:ILE:CD1	0.55	2.67	57	4
1:B:173:ARG:O	1:B:173:ARG:NE	0.55	2.40	98	2
1:A:35:GLU:OE2	1:B:204:ALA:HB2	0.55	2.01	86	1
1:B:76:GLU:OE2	1:B:132:ARG:NH2	0.55	2.40	86	5
1:B:150:ILE:HG23	1:B:175:GLU:OE2	0.55	2.02	39	1
1:B:175:GLU:OE1	1:B:175:GLU:CA	0.55	2.55	12	4
1:A:92:ALA:HB3	1:A:95:GLN:HG2	0.55	1.79	31	10
1:B:140:LYS:NZ	1:B:143:ARG:HH21	0.55	2.00	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:150:ILE:O	1:B:153:ILE:N	0.55	2.26	64	1
1:A:41:SER:CB	1:B:203:LYS:O	0.55	2.55	70	1
1:B:150:ILE:HG23	1:B:151:LEU:HD22	0.55	1.78	85	1
1:B:81:ASP:OD2	1:B:100:ARG:NH2	0.54	2.40	20	2
1:B:144:MET:O	1:B:145:TYR:CG	0.54	2.60	20	1
1:A:100:ARG:HG3	1:A:101:GLY:N	0.54	2.17	47	4
1:B:155:GLN:NE2	1:B:195:ASN:ND2	0.54	2.56	87	3
1:A:76:GLU:OE1	1:A:133:TRP:CZ2	0.54	2.60	24	16
1:B:96:MET:SD	1:B:120:HIS:CE1	0.54	3.00	27	5
1:B:96:MET:SD	1:B:97:ARG:O	0.54	2.65	95	6
1:A:179:GLN:NE2	1:A:182:LYS:NZ	0.54	2.56	69	4
1:B:87:HIS:H	1:B:97:ARG:HH22	0.54	1.45	59	5
1:A:12:HIS:CD2	1:A:12:HIS:H	0.54	2.19	86	6
1:B:5:ASN:HD22	1:B:6:LEU:H	0.54	1.46	90	6
1:A:175:GLU:CD	1:A:176:GLN:N	0.54	2.65	42	15
1:B:95:GLN:CG	1:B:96:MET:N	0.54	2.70	7	7
1:A:37:ILE:HB	1:A:38:PRO:HD3	0.54	1.79	88	4
1:A:16:SER:OG	1:A:18:ARG:NH1	0.54	2.40	96	4
1:A:37:ILE:CD1	1:A:139:ASN:ND2	0.54	2.70	51	1
1:A:7:GLN:N	1:A:7:GLN:CD	0.54	2.66	70	5
1:A:177:ALA:O	1:A:182:LYS:NZ	0.54	2.40	99	2
1:A:4:GLN:NE2	1:A:10:MET:SD	0.54	2.80	88	1
1:A:189:LEU:HD21	1:A:193:ASN:ND2	0.54	2.17	92	3
1:B:98:GLU:H	1:B:98:GLU:CD	0.54	2.10	14	7
1:B:63:GLN:OE1	1:B:67:GLN:NE2	0.54	2.39	28	1
1:A:12:HIS:CE1	1:A:112:GLN:HE22	0.54	2.20	96	3
1:B:7:GLN:N	1:B:7:GLN:CD	0.54	2.66	100	3
1:B:9:GLN:H	1:B:9:GLN:CD	0.54	2.11	89	1
1:B:166:ASP:OD1	1:B:166:ASP:C	0.54	2.50	98	14
1:A:139:ASN:HD22	1:A:167:ARG:NH1	0.54	1.99	3	1
1:B:83:LEU:HD23	1:B:83:LEU:O	0.54	2.03	95	10
1:B:84:HIS:O	1:B:100:ARG:NH1	0.54	2.40	11	13
1:B:78:ALA:O	1:B:81:ASP:OD1	0.54	2.26	59	4
1:A:4:GLN:OE1	1:A:9:GLN:C	0.54	2.51	6	17
1:A:175:GLU:OE1	1:A:185:MET:HE1	0.54	2.03	1	21
1:A:95:GLN:CD	1:A:96:MET:N	0.54	2.66	37	7
1:B:86:VAL:HG12	1:B:100:ARG:HH11	0.54	1.62	82	6
1:B:142:VAL:O	1:B:145:TYR:CD2	0.54	2.60	40	2
1:A:61:GLY:O	1:A:158:LYS:NZ	0.54	2.40	92	1
1:A:79:GLU:OE2	1:A:82:ARG:NH1	0.54	2.41	100	2
1:A:205:LEU:HD13	1:A:213:GLU:OE1	0.54	2.02	17	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:GLN:H	1:A:114:GLN:HE22	0.54	1.45	8	6
1:B:154:ARG:CZ	1:B:155:GLN:O	0.54	2.56	87	4
1:A:203:LYS:HZ2	1:B:38:PRO:CG	0.54	2.15	35	1
1:B:7:GLN:CG	1:B:7:GLN:O	0.54	2.56	48	2
1:A:86:VAL:HG13	1:A:97:ARG:NH2	0.54	2.18	74	2
1:A:100:ARG:HH22	1:A:108:THR:CG2	0.54	2.14	84	1
1:B:25:LYS:O	1:B:29:GLU:OE1	0.54	2.26	84	20
1:B:95:GLN:CD	1:B:96:MET:N	0.54	2.66	65	7
1:A:192:GLN:O	1:A:192:GLN:NE2	0.54	2.41	69	7
1:B:98:GLU:CD	1:B:100:ARG:NH2	0.54	2.66	15	1
1:B:87:HIS:O	1:B:87:HIS:CG	0.54	2.60	46	9
1:B:92:ALA:HB3	1:B:95:GLN:HG2	0.54	1.79	47	5
1:A:5:ASN:HD22	1:A:7:GLN:HE22	0.54	1.46	53	2
1:B:86:VAL:HG23	1:B:100:ARG:HH21	0.54	1.63	96	2
1:B:5:ASN:OD1	1:B:7:GLN:NE2	0.54	2.40	100	2
1:B:163:ASP:OD1	1:B:167:ARG:NH1	0.54	2.41	66	5
1:B:76:GLU:OE1	1:B:133:TRP:CZ2	0.54	2.61	47	16
1:A:71:GLU:N	1:A:71:GLU:OE1	0.54	2.41	88	3
1:A:155:GLN:NE2	1:A:195:ASN:H	0.54	2.01	78	5
1:B:74:ASN:OD1	1:B:74:ASN:C	0.53	2.52	4	7
1:A:44:SER:O	1:A:131:LYS:NZ	0.53	2.41	25	15
1:A:171:THR:O	1:A:175:GLU:CD	0.53	2.51	60	13
1:B:160:PRO:O	1:B:163:ASP:OD2	0.53	2.25	48	7
1:B:143:ARG:HE	1:B:143:ARG:C	0.53	2.10	87	1
1:A:12:HIS:NE2	1:A:111:LEU:HD11	0.53	2.18	16	26
1:A:50:GLN:O	1:A:53:ASN:OD1	0.53	2.26	22	27
1:B:118:MET:SD	1:B:118:MET:O	0.53	2.67	85	22
1:A:75:GLU:O	1:A:79:GLU:CD	0.53	2.52	39	8
1:A:145:TYR:C	1:A:145:TYR:CD1	0.53	2.83	18	2
1:B:192:GLN:O	1:B:199:LYS:NZ	0.53	2.41	78	3
1:B:155:GLN:OE1	1:B:195:ASN:ND2	0.53	2.42	51	8
1:B:81:ASP:OD1	1:B:100:ARG:NH2	0.53	2.41	99	1
1:B:215:MET:C	1:B:215:MET:SD	0.53	2.92	52	8
1:A:154:ARG:NH1	1:A:195:ASN:OD1	0.53	2.41	99	2
1:B:5:ASN:OD1	1:B:9:GLN:NE2	0.53	2.41	66	2
1:B:113:GLU:CD	1:B:117:TRP:CH2	0.53	2.86	68	1
1:B:95:GLN:C	1:B:96:MET:SD	0.53	2.91	78	23
1:B:171:THR:O	1:B:175:GLU:OE1	0.53	2.27	8	11
1:B:12:HIS:CD2	1:B:111:LEU:CD1	0.53	2.91	14	14
1:B:192:GLN:O	1:B:192:GLN:NE2	0.53	2.42	51	8
1:B:10:MET:SD	1:B:10:MET:O	0.53	2.67	62	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:113:GLU:N	1:B:113:GLU:OE1	0.53	2.42	52	2
1:B:81:ASP:CG	1:B:100:ARG:NH2	0.53	2.66	53	1
1:A:12:HIS:CD2	1:A:111:LEU:CD1	0.53	2.91	16	26
1:B:75:GLU:O	1:B:79:GLU:CD	0.53	2.51	85	13
1:A:23:TRP:CD1	1:A:55:MET:SD	0.53	3.01	72	15
1:A:5:ASN:ND2	1:A:7:GLN:CD	0.53	2.67	61	4
1:A:7:GLN:CB	1:A:9:GLN:HE22	0.53	2.17	69	4
1:B:81:ASP:OD1	1:B:81:ASP:C	0.53	2.51	49	8
1:B:142:VAL:O	1:B:145:TYR:CG	0.53	2.62	40	1
1:A:172:LEU:CD2	1:A:185:MET:SD	0.53	2.97	68	1
1:B:95:GLN:O	1:B:96:MET:SD	0.53	2.66	52	12
1:A:12:HIS:NE2	1:A:50:GLN:OE1	0.53	2.42	14	5
1:A:7:GLN:CD	1:A:9:GLN:OE1	0.53	2.52	72	6
1:A:7:GLN:O	1:A:7:GLN:CD	0.53	2.52	58	8
1:A:7:GLN:CD	1:A:7:GLN:H	0.53	2.12	70	3
1:B:5:ASN:CG	1:B:7:GLN:NE2	0.53	2.67	100	2
1:B:68:MET:SD	1:B:68:MET:O	0.53	2.67	41	12
1:B:98:GLU:OE1	1:B:99:PRO:O	0.53	2.26	8	26
1:B:12:HIS:NE2	1:B:111:LEU:HD11	0.53	2.19	94	17
1:A:97:ARG:CZ	1:A:98:GLU:OE2	0.53	2.57	12	3
1:B:120:HIS:CD2	1:B:121:ASN:H	0.53	2.22	25	5
1:B:173:ARG:O	1:B:173:ARG:CZ	0.53	2.57	67	3
1:A:113:GLU:CD	1:A:117:TRP:CH2	0.53	2.87	12	3
1:A:143:ARG:CD	1:A:154:ARG:O	0.53	2.56	17	1
1:B:99:PRO:C	1:B:100:ARG:HE	0.53	2.11	68	5
1:B:75:GLU:OE1	1:B:76:GLU:OE2	0.53	2.27	73	9
1:A:32:PHE:CZ	1:A:145:TYR:CE1	0.53	2.97	72	1
1:B:32:PHE:O	1:B:145:TYR:CE1	0.53	2.61	100	1
1:A:141:ILE:O	1:A:144:MET:HG2	0.53	2.04	42	6
1:B:80:TRP:CZ3	1:B:84:HIS:CD2	0.53	2.97	11	15
1:B:3:VAL:HG21	1:B:13:GLN:CD	0.53	2.29	13	3
1:A:163:ASP:CG	1:A:167:ARG:NH1	0.53	2.67	56	5
1:A:113:GLU:OE1	1:A:113:GLU:N	0.53	2.42	88	3
1:A:166:ASP:OD2	1:A:167:ARG:NH2	0.53	2.42	57	1
1:A:7:GLN:NE2	1:A:9:GLN:OE1	0.52	2.42	96	5
1:B:7:GLN:O	1:B:7:GLN:CG	0.52	2.56	23	2
1:B:219:GLN:OE1	1:B:219:GLN:O	0.52	2.27	49	4
1:A:5:ASN:ND2	1:A:9:GLN:CG	0.52	2.72	19	7
1:B:95:GLN:CD	1:B:96:MET:H	0.52	2.12	15	6
1:A:95:GLN:C	1:A:96:MET:SD	0.52	2.92	12	4
1:B:91:ILE:N	1:B:91:ILE:CD1	0.52	2.72	24	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:GLU:OE1	1:A:98:GLU:N	0.52	2.42	14	4
1:B:97:ARG:NE	1:B:98:GLU:OE2	0.52	2.43	14	1
1:B:164:TYR:OH	1:B:193:ASN:CG	0.52	2.53	34	3
1:A:139:ASN:ND2	1:A:167:ARG:HE	0.52	2.02	38	1
1:A:75:GLU:OE1	1:A:76:GLU:CD	0.52	2.52	66	2
1:B:86:VAL:CG1	1:B:100:ARG:NH1	0.52	2.73	98	5
1:B:155:GLN:HE22	1:B:195:ASN:CG	0.52	2.13	24	4
1:A:67:GLN:OE1	1:A:68:MET:SD	0.52	2.67	89	3
1:A:32:PHE:CE1	1:A:145:TYR:CE2	0.52	2.97	64	1
1:A:97:ARG:HH11	1:A:100:ARG:NH2	0.52	2.03	75	1
1:B:143:ARG:HH12	1:B:152:ASP:CG	0.52	2.13	100	1
1:B:84:HIS:O	1:B:100:ARG:CZ	0.52	2.58	72	9
1:B:12:HIS:CE1	1:B:50:GLN:NE2	0.52	2.78	22	10
1:B:155:GLN:N	1:B:164:TYR:CE1	0.52	2.78	67	3
1:A:202:LEU:HD21	1:A:214:MET:HE2	0.52	1.81	54	2
1:B:143:ARG:NH1	1:B:152:ASP:OD2	0.52	2.43	100	1
1:A:142:VAL:O	1:A:145:TYR:O	0.52	2.27	9	4
1:B:92:ALA:HB3	1:B:95:GLN:HE21	0.52	1.65	5	14
1:B:44:SER:OG	1:B:131:LYS:NZ	0.52	2.41	82	10
1:B:152:ASP:OD1	1:B:152:ASP:O	0.52	2.28	44	3
1:B:213:GLU:N	1:B:213:GLU:OE1	0.52	2.42	68	3
1:B:5:ASN:ND2	1:B:6:LEU:N	0.52	2.58	90	6
1:A:9:GLN:H	1:A:9:GLN:CD	0.52	2.12	89	3
1:B:7:GLN:HB3	1:B:9:GLN:HE22	0.52	1.65	79	3
1:A:177:ALA:H	1:A:182:LYS:NZ	0.52	2.01	99	2
1:A:12:HIS:CE1	1:A:50:GLN:OE1	0.52	2.63	25	8
1:B:72:THR:O	1:B:76:GLU:OE1	0.52	2.27	11	12
1:A:67:GLN:NE2	1:A:68:MET:SD	0.52	2.83	84	3
1:A:7:GLN:NE2	1:A:7:GLN:H	0.52	2.03	52	2
1:B:113:GLU:OE2	1:B:117:TRP:CH2	0.52	2.62	68	1
1:B:63:GLN:CD	1:B:64:ALA:H	0.52	2.12	1	13
1:A:80:TRP:CH2	1:A:84:HIS:NE2	0.52	2.78	77	26
1:A:140:LYS:NZ	1:A:143:ARG:HH21	0.52	2.02	94	2
1:B:175:GLU:CD	1:B:176:GLN:N	0.52	2.68	68	6
1:A:179:GLN:CD	1:A:182:LYS:NZ	0.52	2.68	23	4
1:B:150:ILE:HD11	1:B:168:PHE:CZ	0.52	2.40	34	2
1:A:142:VAL:O	1:A:145:TYR:CD1	0.52	2.63	44	1
1:B:108:THR:O	1:B:108:THR:CG2	0.52	2.57	73	32
1:A:79:GLU:OE1	1:A:82:ARG:NH1	0.52	2.43	49	3
1:B:139:ASN:HB3	1:B:167:ARG:NH1	0.52	2.19	51	1
1:A:97:ARG:HH21	1:A:100:ARG:HH22	0.52	1.47	61	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:GLU:CD	1:A:100:ARG:NH2	0.52	2.66	85	1
1:A:155:GLN:HE21	1:A:195:ASN:H	0.52	1.47	93	6
1:A:113:GLU:OE1	1:A:117:TRP:CE3	0.52	2.63	14	3
1:A:124:ILE:HD12	1:A:124:ILE:N	0.52	2.20	14	18
1:B:12:HIS:NE2	1:B:48:THR:CG2	0.52	2.73	22	4
1:B:98:GLU:OE1	1:B:98:GLU:N	0.52	2.43	23	6
1:A:121:ASN:O	1:A:121:ASN:CG	0.52	2.53	90	8
1:B:155:GLN:HE21	1:B:195:ASN:H	0.52	1.46	35	6
1:B:66:MET:C	1:B:66:MET:SD	0.52	2.93	10	17
1:A:20:LEU:HD11	1:A:58:THR:CG2	0.52	2.35	74	4
1:A:25:LYS:NZ	1:A:29:GLU:OE2	0.52	2.42	87	3
1:B:20:LEU:HD11	1:B:58:THR:CG2	0.52	2.35	52	4
1:B:4:GLN:OE1	1:B:10:MET:HE1	0.52	2.05	97	1
1:A:205:LEU:CD1	1:A:214:MET:SD	0.51	2.98	2	7
1:A:66:MET:C	1:A:66:MET:SD	0.51	2.93	39	29
1:B:12:HIS:CD2	1:B:111:LEU:HD21	0.51	2.39	52	10
1:B:150:ILE:O	1:B:153:ILE:HG22	0.51	2.06	28	8
1:B:7:GLN:CB	1:B:9:GLN:HE22	0.51	2.18	34	8
1:A:150:ILE:O	1:A:153:ILE:HG22	0.51	2.05	87	3
1:A:150:ILE:HD11	1:A:168:PHE:CE1	0.51	2.41	86	2
1:A:99:PRO:O	1:A:100:ARG:NH2	0.51	2.43	64	1
1:B:91:ILE:HD11	1:B:97:ARG:NH1	0.51	2.20	79	2
1:B:92:ALA:HB3	1:B:95:GLN:CD	0.51	2.30	75	13
1:B:113:GLU:OE1	1:B:117:TRP:CE3	0.51	2.63	64	2
1:A:10:MET:SD	1:A:10:MET:O	0.51	2.68	49	4
1:A:12:HIS:CE1	1:A:50:GLN:HE22	0.51	2.23	7	6
1:A:167:ARG:NH2	1:A:170:LYS:CG	0.51	2.73	83	3
1:B:143:ARG:CZ	1:B:144:MET:SD	0.51	2.99	4	6
1:B:167:ARG:HA	1:B:167:ARG:NE	0.51	2.21	8	2
1:B:15:ILE:O	1:B:15:ILE:HD12	0.51	2.06	23	4
1:A:184:TRP:CH2	1:B:184:TRP:CZ3	0.51	2.98	100	6
1:A:118:MET:SD	1:A:118:MET:O	0.51	2.69	67	4
1:A:139:ASN:ND2	1:A:143:ARG:HH12	0.51	2.02	28	1
1:A:192:GLN:C	1:A:192:GLN:NE2	0.51	2.69	89	6
1:B:132:ARG:NH2	1:B:133:TRP:NE1	0.51	2.58	70	1
1:B:75:GLU:O	1:B:79:GLU:OE1	0.51	2.29	6	17
1:B:132:ARG:O	1:B:136:LEU:HD13	0.51	2.06	8	10
1:B:139:ASN:ND2	1:B:143:ARG:HH11	0.51	2.03	46	1
1:B:143:ARG:CG	1:B:167:ARG:HH12	0.51	2.18	51	1
1:A:181:VAL:HG22	1:B:180:GLU:O	0.51	2.05	67	84
1:B:75:GLU:OE2	1:B:79:GLU:OE2	0.51	2.29	45	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:205:LEU:HD12	1:A:214:MET:SD	0.51	2.45	2	7
1:A:12:HIS:HB3	1:A:115:ILE:HD11	0.51	1.83	93	29
1:B:145:TYR:C	1:B:145:TYR:CD1	0.51	2.87	80	3
1:B:86:VAL:N	1:B:100:ARG:NH1	0.51	2.59	72	9
1:B:139:ASN:HD22	1:B:170:LYS:NZ	0.51	2.04	38	1
1:B:64:ALA:O	1:B:68:MET:SD	0.51	2.69	53	5
1:B:154:ARG:C	1:B:154:ARG:HE	0.51	2.14	94	1
1:B:150:ILE:HD11	1:B:168:PHE:CE1	0.51	2.41	50	3
1:A:144:MET:C	1:A:145:TYR:CG	0.51	2.89	56	2
1:B:150:ILE:CD1	1:B:151:LEU:H	0.51	2.19	67	1
1:B:118:MET:SD	1:B:118:MET:C	0.51	2.94	85	18
1:A:32:PHE:CD1	1:A:145:TYR:CD2	0.51	2.99	10	1
1:B:5:ASN:ND2	1:B:7:GLN:OE1	0.51	2.44	61	2
1:B:98:GLU:CD	1:B:100:ARG:HH21	0.51	2.14	11	6
1:A:4:GLN:N	1:A:4:GLN:CD	0.51	2.69	12	1
1:B:97:ARG:CZ	1:B:98:GLU:OE1	0.51	2.59	32	2
1:B:139:ASN:OD1	1:B:143:ARG:NE	0.51	2.43	52	1
1:A:150:ILE:N	1:A:153:ILE:HG12	0.51	2.21	61	1
1:A:178:SER:OG	1:B:180:GLU:HB3	0.51	2.05	69	1
1:A:153:ILE:O	1:A:153:ILE:HG23	0.51	2.06	78	1
1:A:100:ARG:NH2	1:A:108:THR:CG2	0.51	2.74	84	1
1:A:4:GLN:CD	1:A:4:GLN:O	0.51	2.54	82	4
1:A:12:HIS:CG	1:A:111:LEU:HD11	0.51	2.40	82	10
1:A:96:MET:CE	1:A:120:HIS:NE2	0.51	2.74	89	8
1:B:202:LEU:HD21	1:B:214:MET:HE2	0.51	1.83	18	4
1:A:176:GLN:NE2	1:A:176:GLN:C	0.51	2.68	20	7
1:B:121:ASN:CG	1:B:121:ASN:O	0.51	2.54	85	15
1:B:177:ALA:H	1:B:182:LYS:NZ	0.51	2.03	11	6
1:B:210:THR:OG1	1:B:213:GLU:CD	0.51	2.54	88	15
1:B:76:GLU:CD	1:B:133:TRP:NE1	0.51	2.69	35	9
1:B:167:ARG:NH2	1:B:171:THR:N	0.51	2.59	39	1
1:B:68:MET:HE3	1:B:144:MET:CE	0.51	2.34	51	3
1:B:150:ILE:HG22	1:B:151:LEU:N	0.51	2.17	64	1
1:A:161:PHE:CE1	1:A:198:CYS:SG	0.51	3.04	69	10
1:B:63:GLN:CD	1:B:63:GLN:H	0.51	2.05	85	2
1:A:76:GLU:CD	1:A:76:GLU:N	0.50	2.69	84	7
1:A:81:ASP:OD2	1:A:100:ARG:NH2	0.50	2.44	51	3
1:A:67:GLN:OE1	1:A:68:MET:CE	0.50	2.59	34	3
1:B:67:GLN:O	1:B:71:GLU:OE1	0.50	2.29	54	2
1:A:100:ARG:NE	1:A:101:GLY:H	0.50	2.03	57	2
1:A:32:PHE:CD1	1:A:145:TYR:CE2	0.50	2.99	64	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:ILE:HD11	1:A:172:LEU:CA	0.50	2.34	78	1
1:A:139:ASN:ND2	1:A:143:ARG:CZ	0.50	2.74	97	1
1:A:4:GLN:HE22	1:A:10:MET:HE3	0.50	1.66	40	5
1:B:198:CYS:SG	1:B:202:LEU:HD11	0.50	2.47	68	77
1:A:25:LYS:O	1:A:29:GLU:OE1	0.50	2.30	82	10
1:A:4:GLN:OE1	1:A:10:MET:SD	0.50	2.70	92	3
1:A:175:GLU:OE1	1:A:175:GLU:CA	0.50	2.59	51	8
1:A:180:GLU:OE1	1:A:183:ASN:ND2	0.50	2.44	72	8
1:A:203:LYS:NZ	1:B:34:PRO:O	0.50	2.39	35	1
1:A:67:GLN:O	1:A:71:GLU:OE1	0.50	2.29	51	6
1:B:136:LEU:HA	1:B:167:ARG:NH1	0.50	2.21	8	1
1:B:75:GLU:CD	1:B:75:GLU:C	0.50	2.79	55	11
1:A:108:THR:O	1:A:108:THR:CG2	0.50	2.59	57	17
1:B:95:GLN:OE1	1:B:96:MET:N	0.50	2.44	68	2
1:B:7:GLN:C	1:B:9:GLN:HE22	0.50	2.14	15	6
1:A:215:MET:C	1:A:215:MET:SD	0.50	2.94	86	12
1:A:171:THR:HG22	1:A:175:GLU:OE2	0.50	2.07	100	4
1:B:35:GLU:OE2	1:B:39:MET:SD	0.50	2.69	54	2
1:A:4:GLN:CD	1:A:10:MET:SD	0.50	2.95	62	2
1:A:172:LEU:C	1:A:172:LEU:CD1	0.50	2.84	68	1
1:A:98:GLU:OE2	1:A:100:ARG:NH2	0.50	2.44	91	1
1:B:81:ASP:OD1	1:B:82:ARG:CZ	0.50	2.60	100	1
1:A:2:ILE:N	1:A:2:ILE:CD1	0.50	2.73	42	24
1:A:195:ASN:OD1	1:A:195:ASN:C	0.50	2.54	57	52
1:B:150:ILE:CG2	1:B:151:LEU:N	0.50	2.75	94	9
1:B:34:PRO:CB	1:B:152:ASP:OD1	0.50	2.59	28	1
1:A:173:ARG:O	1:A:173:ARG:NE	0.50	2.43	32	2
1:A:177:ALA:HB3	1:A:182:LYS:HZ1	0.50	1.67	54	2
1:A:4:GLN:CD	1:A:4:GLN:N	0.50	2.69	62	1
1:A:20:LEU:C	1:A:20:LEU:CD2	0.50	2.85	42	7
1:B:118:MET:C	1:B:118:MET:SD	0.50	2.95	24	8
1:B:179:GLN:NE2	1:B:179:GLN:H	0.50	2.03	46	5
1:A:4:GLN:OE1	1:A:10:MET:CA	0.50	2.60	96	4
1:B:15:ILE:CD1	1:B:55:MET:SD	0.50	3.00	67	1
1:A:41:SER:O	1:B:204:ALA:HA	0.50	2.07	70	1
1:A:144:MET:C	1:A:144:MET:SD	0.50	2.95	66	9
1:A:72:THR:O	1:A:76:GLU:OE1	0.50	2.30	62	11
1:A:75:GLU:OE1	1:A:76:GLU:OE2	0.50	2.29	22	8
1:A:162:ARG:HH21	1:A:215:MET:CE	0.50	2.19	43	4
1:A:76:GLU:OE2	1:A:132:ARG:NH2	0.50	2.45	55	1
1:A:11:VAL:CG2	1:A:12:HIS:N	0.50	2.75	6	29

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:GLU:O	1:A:74:ASN:OD1	0.50	2.30	26	14
1:A:145:TYR:O	1:A:145:TYR:CD2	0.50	2.65	83	2
1:B:2:ILE:HD12	1:B:118:MET:SD	0.50	2.46	32	4
1:A:69:LEU:HD21	1:A:138:LEU:HD12	0.50	1.83	78	10
1:A:75:GLU:O	1:A:79:GLU:OE1	0.50	2.30	98	8
1:A:120:HIS:ND1	1:A:121:ASN:N	0.50	2.60	76	21
1:B:176:GLN:N	1:B:176:GLN:CD	0.50	2.70	62	3
1:B:150:ILE:HD13	1:B:185:MET:SD	0.50	2.47	73	2
1:B:143:ARG:HH12	1:B:154:ARG:HE	0.50	1.49	66	1
1:B:100:ARG:HH21	1:B:102:SER:N	0.50	2.05	77	2
1:B:120:HIS:CD2	1:B:122:PRO:O	0.50	2.65	85	2
1:A:159:GLU:OE2	1:A:163:ASP:CG	0.50	2.55	37	3
1:A:183:ASN:OD1	1:A:183:ASN:C	0.50	2.50	27	7
1:B:171:THR:O	1:B:175:GLU:CD	0.50	2.55	92	16
1:B:11:VAL:CG1	1:B:12:HIS:N	0.50	2.75	84	27
1:A:87:HIS:O	1:A:97:ARG:CZ	0.50	2.60	13	6
1:B:139:ASN:OD1	1:B:143:ARG:CZ	0.50	2.59	88	3
1:A:2:ILE:HG22	1:A:115:ILE:CD1	0.50	2.37	52	2
1:A:144:MET:HB3	1:A:145:TYR:CE2	0.50	2.41	78	2
1:A:7:GLN:C	1:A:9:GLN:HE22	0.50	2.14	69	1
1:A:179:GLN:N	1:A:179:GLN:OE1	0.50	2.43	96	1
1:A:103:ASP:CG	1:A:109:SER:OG	0.49	2.55	90	16
1:B:197:ASP:OD1	1:B:197:ASP:N	0.49	2.44	63	3
1:B:63:GLN:O	1:B:63:GLN:OE1	0.49	2.30	76	4
1:B:144:MET:C	1:B:145:TYR:O	0.49	2.55	73	2
1:A:180:GLU:HB2	1:B:180:GLU:CB	0.49	2.36	1	100
1:A:198:CYS:SG	1:A:202:LEU:CD1	0.49	3.00	42	92
1:A:5:ASN:CG	1:A:7:GLN:H	0.49	2.16	37	9
1:B:195:ASN:OD1	1:B:195:ASN:C	0.49	2.55	77	45
1:B:196:PRO:O	1:B:200:THR:HG23	0.49	2.06	66	40
1:B:34:PRO:HB2	1:B:152:ASP:OD1	0.49	2.06	28	1
1:B:81:ASP:OD1	1:B:81:ASP:O	0.49	2.31	17	46
1:B:28:GLU:OE1	1:B:29:GLU:CD	0.49	2.55	29	7
1:A:84:HIS:CD2	1:A:98:GLU:CD	0.49	2.91	74	3
1:A:167:ARG:NE	1:A:167:ARG:HA	0.49	2.22	51	1
1:A:172:LEU:HD13	1:A:172:LEU:O	0.49	2.06	68	1
1:A:11:VAL:CG1	1:A:12:HIS:N	0.49	2.76	93	28
1:B:9:GLN:N	1:B:9:GLN:OE1	0.49	2.45	63	2
1:B:4:GLN:OE1	1:B:8:GLY:O	0.49	2.31	71	7
1:A:110:THR:OG1	1:A:113:GLU:OE1	0.49	2.29	78	3
1:B:54:THR:O	1:B:57:ASN:OD1	0.49	2.30	97	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:97:ARG:HE	1:B:100:ARG:HH22	0.49	1.50	62	1
1:A:140:LYS:HZ3	1:A:143:ARG:HH21	0.49	1.48	94	1
1:A:6:LEU:O	1:A:6:LEU:HD13	0.49	2.08	81	9
1:B:67:GLN:CD	1:B:67:GLN:C	0.49	2.80	40	15
1:B:85:PRO:O	1:B:87:HIS:NE2	0.49	2.46	37	2
1:A:18:ARG:O	1:A:18:ARG:NE	0.49	2.46	93	3
1:A:155:GLN:OE1	1:A:195:ASN:ND2	0.49	2.45	14	3
1:A:167:ARG:HH21	1:A:171:THR:CA	0.49	2.20	31	1
1:B:145:TYR:CD2	1:B:145:TYR:O	0.49	2.66	43	1
1:B:94:GLY:C	1:B:95:GLN:NE2	0.49	2.70	26	12
1:A:95:GLN:CD	1:A:96:MET:H	0.49	2.16	27	7
1:A:171:THR:O	1:A:175:GLU:OE2	0.49	2.30	51	16
1:B:97:ARG:HH12	1:B:100:ARG:CZ	0.49	2.21	97	1
1:A:178:SER:OG	1:B:180:GLU:CG	0.49	2.60	12	56
1:A:18:ARG:NH1	1:A:21:ASN:HD22	0.49	2.05	93	2
1:A:210:THR:HG1	1:A:213:GLU:CD	0.49	2.16	19	1
1:B:143:ARG:NE	1:B:143:ARG:HA	0.49	2.22	27	1
1:B:154:ARG:HE	1:B:155:GLN:C	0.49	2.15	64	2
1:A:69:LEU:HD21	1:A:138:LEU:CD1	0.49	2.38	33	10
1:A:92:ALA:HB3	1:A:95:GLN:CD	0.49	2.33	62	6
1:A:98:GLU:OE1	1:A:99:PRO:O	0.49	2.30	49	14
1:B:32:PHE:CE1	1:B:145:TYR:CG	0.49	3.01	18	1
1:A:175:GLU:OE1	1:A:177:ALA:CB	0.49	2.61	67	1
1:A:203:LYS:CE	1:B:139:ASN:CG	0.49	2.86	80	1
1:B:167:ARG:NH1	1:B:171:THR:HG22	0.49	2.23	17	4
1:B:192:GLN:NE2	1:B:192:GLN:C	0.49	2.70	51	14
1:B:171:THR:HG22	1:B:175:GLU:OE2	0.49	2.06	51	4
1:A:2:ILE:HD13	1:A:2:ILE:N	0.49	2.23	6	17
1:A:97:ARG:HE	1:A:100:ARG:CZ	0.49	2.21	12	3
1:B:87:HIS:O	1:B:97:ARG:CZ	0.49	2.61	12	2
1:A:219:GLN:O	1:A:219:GLN:OE1	0.48	2.30	81	8
1:B:185:MET:SD	1:B:185:MET:N	0.48	2.86	51	10
1:A:80:TRP:CZ3	1:A:84:HIS:CD2	0.48	3.01	70	6
1:B:96:MET:SD	1:B:120:HIS:CD2	0.48	3.06	14	11
1:A:15:ILE:CD1	1:A:55:MET:SD	0.48	3.01	21	8
1:B:78:ALA:C	1:B:82:ARG:NH1	0.48	2.71	25	2
1:A:37:ILE:HD13	1:A:139:ASN:ND2	0.48	2.23	33	4
1:B:139:ASN:HD22	1:B:170:LYS:HE3	0.48	1.66	43	1
1:B:18:ARG:HH21	1:B:22:ALA:N	0.48	2.05	68	1
1:A:32:PHE:CE2	1:A:145:TYR:CE2	0.48	3.01	86	1
1:A:7:GLN:HE22	1:A:9:GLN:CD	0.48	2.16	100	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:219:GLN:OE1	1:A:219:GLN:C	0.48	2.56	85	14
1:A:67:GLN:CD	1:A:67:GLN:C	0.48	2.81	84	7
1:B:103:ASP:CG	1:B:109:SER:OG	0.48	2.56	92	7
1:A:150:ILE:HG13	1:A:151:LEU:H	0.48	1.68	65	2
1:A:7:GLN:O	1:A:7:GLN:CG	0.48	2.61	58	6
1:A:120:HIS:CD2	1:A:121:ASN:H	0.48	2.25	91	3
1:A:96:MET:SD	1:A:120:HIS:ND1	0.48	2.86	52	4
1:A:163:ASP:OD1	1:A:167:ARG:CZ	0.48	2.60	52	1
1:B:110:THR:OG1	1:B:113:GLU:CD	0.48	2.56	52	2
1:B:2:ILE:HD13	1:B:118:MET:HE3	0.48	1.86	68	1
1:A:153:ILE:N	1:A:153:ILE:CD1	0.48	2.76	44	7
1:B:25:LYS:NZ	1:B:29:GLU:OE1	0.48	2.46	18	3
1:A:179:GLN:CD	1:A:182:LYS:HZ1	0.48	2.17	58	2
1:A:150:ILE:CG1	1:A:151:LEU:N	0.48	2.73	94	1
1:A:4:GLN:CD	1:A:8:GLY:O	0.48	2.56	85	11
1:A:34:PRO:O	1:B:203:LYS:NZ	0.48	2.47	96	1
1:A:154:ARG:NH1	1:A:155:GLN:O	0.48	2.46	5	8
1:B:2:ILE:CD1	1:B:118:MET:SD	0.48	3.02	41	16
1:A:103:ASP:CB	1:A:109:SER:OG	0.48	2.62	35	16
1:A:133:TRP:CD1	1:A:133:TRP:N	0.48	2.81	93	15
1:A:150:ILE:H	1:A:171:THR:HG21	0.48	1.69	6	1
1:A:113:GLU:OE2	1:A:117:TRP:CH2	0.48	2.66	92	5
1:B:9:GLN:CD	1:B:9:GLN:H	0.48	2.16	34	2
1:B:50:GLN:NE2	1:B:54:THR:OG1	0.48	2.47	39	1
1:B:139:ASN:HD21	1:B:143:ARG:HH11	0.48	1.51	46	2
1:A:143:ARG:NH1	1:A:153:ILE:HD11	0.48	2.23	51	1
1:A:66:MET:HE1	1:A:67:GLN:HE21	0.48	1.67	69	1
1:A:150:ILE:C	1:A:150:ILE:CD1	0.48	2.85	86	1
1:B:103:ASP:CB	1:B:109:SER:OG	0.48	2.62	55	7
1:B:156:GLY:H	1:B:159:GLU:CD	0.48	2.16	14	5
1:B:2:ILE:N	1:B:2:ILE:CD1	0.48	2.74	69	1
1:A:180:GLU:O	1:B:181:VAL:HG22	0.48	2.08	50	55
1:B:50:GLN:H	1:B:114:GLN:HE22	0.48	1.51	62	4
1:A:113:GLU:O	1:A:113:GLU:OE1	0.48	2.31	64	2
1:A:4:GLN:OE1	1:A:5:ASN:O	0.48	2.32	23	6
1:A:50:GLN:NE2	1:A:54:THR:OG1	0.48	2.47	12	4
1:B:99:PRO:O	1:B:100:ARG:NH2	0.48	2.46	33	1
1:A:91:ILE:HD12	1:A:97:ARG:NH2	0.48	2.24	87	1
1:A:210:THR:OG1	1:A:213:GLU:CD	0.48	2.57	76	7
1:A:213:GLU:OE1	1:A:213:GLU:N	0.48	2.47	39	9
1:A:32:PHE:CZ	1:A:145:TYR:CE2	0.48	3.02	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:194:ALA:HB1	1:B:198:CYS:SG	0.48	2.49	22	4
1:B:145:TYR:O	1:B:145:TYR:CG	0.48	2.67	69	2
1:B:32:PHE:CD2	1:B:145:TYR:CE2	0.48	3.02	23	1
1:B:96:MET:HE1	1:B:116:GLY:O	0.48	2.09	23	3
1:A:164:TYR:OH	1:A:193:ASN:CB	0.48	2.62	31	1
1:B:11:VAL:CG2	1:B:12:HIS:N	0.48	2.77	32	7
1:A:143:ARG:NH2	1:A:170:LYS:HZ1	0.48	2.04	43	1
1:A:68:MET:SD	1:A:68:MET:N	0.48	2.87	62	2
1:B:79:GLU:N	1:B:79:GLU:OE1	0.48	2.47	63	1
1:A:39:MET:SD	1:A:39:MET:N	0.47	2.87	46	23
1:B:12:HIS:CD2	1:B:115:ILE:HD11	0.47	2.44	47	4
1:B:71:GLU:O	1:B:75:GLU:CD	0.47	2.57	89	3
1:B:143:ARG:NH1	1:B:152:ASP:CG	0.47	2.72	100	1
1:A:110:THR:HG22	1:A:111:LEU:N	0.47	2.24	51	24
1:B:57:ASN:OD1	1:B:57:ASN:O	0.47	2.32	27	14
1:B:7:GLN:NE2	1:B:9:GLN:NE2	0.47	2.62	74	3
1:A:97:ARG:HH11	1:A:100:ARG:NH1	0.47	2.07	46	1
1:B:57:ASN:OD1	1:B:57:ASN:C	0.47	2.57	97	2
1:B:72:THR:O	1:B:76:GLU:OE2	0.47	2.32	6	14
1:A:179:GLN:OE1	1:A:182:LYS:NZ	0.47	2.44	23	4
1:A:39:MET:N	1:A:39:MET:SD	0.47	2.87	32	7
1:B:175:GLU:OE1	1:B:185:MET:HE1	0.47	2.09	34	3
1:A:143:ARG:CD	1:A:171:THR:HA	0.47	2.39	43	1
1:A:67:GLN:O	1:A:71:GLU:CD	0.47	2.57	96	4
1:B:20:LEU:CD1	1:B:58:THR:HG21	0.47	2.40	52	4
1:A:18:ARG:CD	1:A:18:ARG:N	0.47	2.76	53	1
1:B:166:ASP:CG	1:B:167:ARG:NH2	0.47	2.72	73	2
1:A:72:THR:O	1:A:76:GLU:OE2	0.47	2.32	84	7
1:A:81:ASP:O	1:A:81:ASP:OD1	0.47	2.33	34	21
1:A:120:HIS:ND1	1:A:122:PRO:O	0.47	2.48	91	4
1:A:7:GLN:CD	1:A:7:GLN:C	0.47	2.81	53	2
1:B:91:ILE:HG21	1:B:97:ARG:NH2	0.47	2.24	54	1
1:A:141:ILE:HG23	1:A:145:TYR:CE2	0.47	2.44	64	1
1:B:143:ARG:C	1:B:143:ARG:NE	0.47	2.73	87	1
1:B:15:ILE:H	1:B:15:ILE:CD1	0.47	2.22	6	16
1:B:5:ASN:HD21	1:B:7:GLN:CD	0.47	2.17	15	2
1:A:162:ARG:CZ	1:A:219:GLN:HE22	0.47	2.22	23	1
1:B:78:ALA:CB	1:B:82:ARG:HH12	0.47	2.22	25	2
1:A:139:ASN:HD22	1:A:167:ARG:HH21	0.47	1.52	28	1
1:B:183:ASN:OD1	1:B:187:GLU:CD	0.47	2.58	81	2
1:A:79:GLU:CD	1:A:82:ARG:HH12	0.47	2.17	55	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:154:ARG:O	1:B:154:ARG:NE	0.47	2.47	94	2
1:B:179:GLN:OE1	1:B:182:LYS:NZ	0.47	2.44	69	1
1:B:96:MET:SD	1:B:97:ARG:NH1	0.47	2.88	99	1
1:B:159:GLU:OE2	1:B:163:ASP:OD2	0.47	2.33	65	8
1:A:210:THR:OG1	1:A:213:GLU:OE1	0.47	2.33	92	7
1:A:12:HIS:C	1:A:13:GLN:NE2	0.47	2.72	14	3
1:B:109:SER:OG	1:B:114:GLN:NE2	0.47	2.48	36	3
1:B:4:GLN:OE1	1:B:5:ASN:O	0.47	2.32	98	6
1:B:16:SER:OG	1:B:18:ARG:NH1	0.47	2.48	96	1
1:A:153:ILE:O	1:A:193:ASN:OD1	0.47	2.32	2	29
1:B:78:ALA:C	1:B:82:ARG:HH21	0.47	2.18	38	5
1:B:17:PRO:O	1:B:21:ASN:OD1	0.47	2.32	84	18
1:A:183:ASN:O	1:A:187:GLU:OE1	0.47	2.33	94	3
1:A:20:LEU:CD1	1:A:58:THR:HG21	0.47	2.40	74	4
1:A:54:THR:O	1:A:57:ASN:OD1	0.47	2.33	52	2
1:B:80:TRP:CE2	1:B:84:HIS:CE1	0.47	3.03	52	1
1:B:110:THR:HG1	1:B:113:GLU:CD	0.47	2.17	52	1
1:A:18:ARG:H	1:A:18:ARG:NE	0.47	2.08	53	1
1:B:153:ILE:N	1:B:153:ILE:HD12	0.47	2.24	99	2
1:B:144:MET:O	1:B:145:TYR:CB	0.47	2.63	61	1
1:A:96:MET:HE1	1:A:116:GLY:O	0.47	2.10	69	1
1:A:21:ASN:O	1:A:24:VAL:HG12	0.47	2.10	85	24
1:B:12:HIS:CG	1:B:111:LEU:CD2	0.47	2.98	45	24
1:B:139:ASN:OD1	1:B:143:ARG:NH2	0.47	2.48	68	1
1:B:175:GLU:OE1	1:B:176:GLN:C	0.47	2.57	68	1
1:B:97:ARG:HE	1:B:100:ARG:NH1	0.47	2.08	90	1
1:B:195:ASN:OD1	1:B:197:ASP:N	0.47	2.48	77	26
1:A:182:LYS:HZ2	1:A:182:LYS:HB2	0.47	1.70	58	3
1:B:150:ILE:HD11	1:B:168:PHE:CD1	0.47	2.44	24	1
1:A:139:ASN:HD22	1:A:167:ARG:NH2	0.47	2.08	28	1
1:A:86:VAL:HG12	1:A:100:ARG:NH1	0.47	2.24	61	3
1:B:143:ARG:HH21	1:B:154:ARG:CZ	0.47	2.23	75	1
1:B:68:MET:SD	1:B:68:MET:C	0.47	2.98	10	11
1:A:219:GLN:O	1:A:219:GLN:CG	0.47	2.63	19	8
1:B:210:THR:OG1	1:B:213:GLU:OE1	0.47	2.33	33	7
1:A:166:ASP:OD1	1:A:166:ASP:C	0.47	2.58	83	13
1:A:80:TRP:CE2	1:A:84:HIS:CD2	0.47	3.03	50	6
1:A:5:ASN:N	1:A:5:ASN:OD1	0.47	2.47	24	2
1:A:75:GLU:CD	1:A:75:GLU:C	0.47	2.83	51	6
1:A:44:SER:CB	1:A:131:LYS:HZ2	0.47	2.23	90	5
1:B:97:ARG:NH1	1:B:98:GLU:OE2	0.47	2.47	53	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:ASN:OD1	1:A:21:ASN:C	0.47	2.57	99	2
1:A:173:ARG:NH2	1:A:182:LYS:NZ	0.47	2.62	69	1
1:B:91:ILE:HD11	1:B:97:ARG:HH11	0.47	1.69	92	1
1:B:13:GLN:OE1	1:B:14:ALA:N	0.47	2.48	95	1
1:A:12:HIS:CG	1:A:111:LEU:CD2	0.46	2.98	8	20
1:A:192:GLN:NE2	1:A:192:GLN:O	0.46	2.48	89	3
1:A:204:ALA:HA	1:B:41:SER:C	0.46	2.35	70	1
1:B:184:TRP:NE1	1:B:188:THR:OG1	0.46	2.48	16	14
1:B:21:ASN:O	1:B:24:VAL:HG12	0.46	2.10	15	16
1:B:110:THR:HG22	1:B:111:LEU:N	0.46	2.25	70	14
1:A:140:LYS:HZ2	1:A:143:ARG:HH22	0.46	1.52	14	1
1:A:97:ARG:HH11	1:A:100:ARG:CZ	0.46	2.24	50	3
1:B:63:GLN:NE2	1:B:64:ALA:CA	0.46	2.78	28	1
1:A:76:GLU:CD	1:A:133:TRP:NE1	0.46	2.73	33	2
1:B:198:CYS:SG	1:B:221:VAL:HG11	0.46	2.50	34	3
1:B:97:ARG:HH21	1:B:100:ARG:HH11	0.46	1.51	90	1
1:A:184:TRP:CZ3	1:B:184:TRP:CH2	0.46	3.03	7	7
1:B:184:TRP:CE3	1:B:185:MET:SD	0.46	3.08	37	7
1:A:192:GLN:NE2	1:A:192:GLN:C	0.46	2.73	69	6
1:A:118:MET:SD	1:A:118:MET:C	0.46	2.98	98	6
1:B:219:GLN:CD	1:B:219:GLN:O	0.46	2.59	15	2
1:B:7:GLN:NE2	1:B:9:GLN:OE1	0.46	2.48	49	3
1:B:167:ARG:O	1:B:167:ARG:NE	0.46	2.46	39	5
1:B:76:GLU:OE1	1:B:76:GLU:C	0.46	2.58	47	11
1:B:192:GLN:NE2	1:B:192:GLN:O	0.46	2.48	55	2
1:A:25:LYS:HZ3	1:A:29:GLU:CD	0.46	2.18	77	2
1:B:71:GLU:OE1	1:B:71:GLU:C	0.46	2.59	46	1
1:A:5:ASN:HD21	1:A:7:GLN:CD	0.46	2.18	61	1
1:B:91:ILE:HD12	1:B:97:ARG:NH2	0.46	2.26	78	1
1:B:5:ASN:OD1	1:B:7:GLN:OE1	0.46	2.33	95	4
1:A:17:PRO:O	1:A:21:ASN:OD1	0.46	2.33	49	5
1:A:80:TRP:CD2	1:A:84:HIS:CD2	0.46	3.04	77	8
1:B:78:ALA:HB1	1:B:82:ARG:HH12	0.46	1.70	46	2
1:A:7:GLN:H	1:A:7:GLN:CD	0.46	2.19	31	6
1:A:57:ASN:O	1:A:57:ASN:OD1	0.46	2.33	89	3
1:B:4:GLN:OE1	1:B:8:GLY:C	0.46	2.59	71	3
1:B:153:ILE:O	1:B:193:ASN:OD1	0.46	2.33	36	20
1:A:69:LEU:HD21	1:A:138:LEU:HD22	0.46	1.88	64	3
1:A:203:LYS:NZ	1:B:38:PRO:CG	0.46	2.79	35	1
1:B:79:GLU:CD	1:B:79:GLU:O	0.46	2.58	54	1
1:A:100:ARG:CD	1:A:101:GLY:N	0.46	2.75	57	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:4:GLN:O	1:B:4:GLN:OE1	0.46	2.34	36	14
1:A:25:LYS:CB	1:A:25:LYS:HZ3	0.46	2.23	7	3
1:A:68:MET:HE3	1:A:144:MET:SD	0.46	2.51	82	5
1:A:113:GLU:OE2	1:A:117:TRP:CZ2	0.46	2.68	14	2
1:B:150:ILE:CG1	1:B:151:LEU:N	0.46	2.78	22	1
1:B:121:ASN:O	1:B:121:ASN:OD1	0.46	2.34	34	5
1:B:76:GLU:N	1:B:76:GLU:CD	0.46	2.74	85	17
1:B:121:ASN:O	1:B:121:ASN:CG	0.46	2.59	86	6
1:A:5:ASN:ND2	1:A:7:GLN:OE1	0.46	2.48	44	5
1:A:139:ASN:ND2	1:A:167:ARG:HG3	0.46	2.25	43	2
1:B:85:PRO:C	1:B:100:ARG:HH12	0.46	2.19	15	2
1:B:4:GLN:OE1	1:B:9:GLN:C	0.46	2.59	56	7
1:A:4:GLN:OE1	1:A:8:GLY:O	0.46	2.34	74	4
1:A:87:HIS:CG	1:A:87:HIS:O	0.46	2.68	29	2
1:A:76:GLU:OE2	1:A:80:TRP:CE3	0.46	2.69	52	1
1:A:18:ARG:N	1:A:18:ARG:NE	0.46	2.64	53	1
1:A:162:ARG:NH2	1:A:215:MET:CE	0.46	2.79	71	2
1:A:163:ASP:CG	1:A:167:ARG:HH12	0.46	2.19	56	2
1:B:39:MET:SD	1:B:39:MET:N	0.46	2.89	96	15
1:B:15:ILE:HD11	1:B:51:ASP:HB3	0.46	1.88	70	26
1:B:98:GLU:OE1	1:B:98:GLU:C	0.46	2.59	66	18
1:A:5:ASN:OD1	1:A:7:GLN:OE1	0.46	2.33	15	3
1:A:20:LEU:HD11	1:A:58:THR:OG1	0.46	2.11	74	11
1:B:179:GLN:N	1:B:179:GLN:CD	0.46	2.74	46	4
1:B:197:ASP:OD1	1:B:198:CYS:N	0.46	2.49	24	4
1:B:199:LYS:NZ	1:B:199:LYS:CB	0.46	2.79	76	6
1:B:5:ASN:CG	1:B:7:GLN:H	0.46	2.18	57	2
1:B:144:MET:O	1:B:145:TYR:HB2	0.46	2.09	61	1
1:A:152:ASP:O	1:A:152:ASP:OD1	0.46	2.34	87	2
1:A:159:GLU:OE2	1:A:163:ASP:OD2	0.46	2.34	37	4
1:A:15:ILE:H	1:A:15:ILE:CD1	0.46	2.23	38	16
1:A:195:ASN:OD1	1:A:197:ASP:N	0.46	2.48	34	30
1:B:69:LEU:HD21	1:B:138:LEU:HD22	0.46	1.88	48	4
1:A:7:GLN:CD	1:A:7:GLN:N	0.46	2.73	31	3
1:A:86:VAL:CG2	1:A:100:ARG:CZ	0.46	2.94	55	1
1:B:150:ILE:O	1:B:152:ASP:N	0.46	2.49	64	1
1:A:150:ILE:O	1:A:151:LEU:C	0.46	2.59	88	1
1:B:76:GLU:OE1	1:B:76:GLU:O	0.45	2.34	72	14
1:B:164:TYR:OH	1:B:193:ASN:CB	0.45	2.64	67	3
1:B:16:SER:OG	1:B:18:ARG:CZ	0.45	2.64	52	1
1:A:2:ILE:CD1	1:A:118:MET:SD	0.45	3.04	98	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:18:ARG:HH21	1:B:21:ASN:CG	0.45	2.19	54	1
1:A:91:ILE:N	1:A:91:ILE:CD1	0.45	2.79	70	2
1:A:95:GLN:N	1:A:95:GLN:CD	0.45	2.74	66	2
1:B:7:GLN:OE1	1:B:7:GLN:O	0.45	2.34	85	14
1:B:50:GLN:CD	1:B:50:GLN:C	0.45	2.83	50	22
1:B:198:CYS:SG	1:B:202:LEU:CD1	0.45	3.04	41	76
1:B:80:TRP:CD2	1:B:84:HIS:CD2	0.45	3.05	23	23
1:B:155:GLN:OE1	1:B:156:GLY:O	0.45	2.34	59	10
1:B:5:ASN:HD22	1:B:6:LEU:N	0.45	2.10	90	5
1:B:193:ASN:OD1	1:B:193:ASN:O	0.45	2.34	89	3
1:A:35:GLU:OE1	1:A:35:GLU:C	0.45	2.60	66	1
1:B:100:ARG:CZ	1:B:102:SER:H	0.45	2.25	83	1
1:A:113:GLU:OE1	1:A:113:GLU:O	0.45	2.34	14	1
1:A:81:ASP:HB3	1:A:100:ARG:NE	0.45	2.26	22	1
1:A:80:TRP:CH2	1:A:84:HIS:CD2	0.45	3.04	27	1
1:B:97:ARG:NH2	1:B:113:GLU:CD	0.45	2.74	66	1
1:B:150:ILE:HD13	1:B:185:MET:HE3	0.45	1.88	76	1
1:B:45:GLU:CD	1:B:45:GLU:O	0.45	2.60	62	3
1:B:85:PRO:C	1:B:100:ARG:HH22	0.45	2.20	72	3
1:B:154:ARG:O	1:B:154:ARG:NH1	0.45	2.49	23	1
1:B:143:ARG:NH1	1:B:167:ARG:HH21	0.45	2.08	37	1
1:A:35:GLU:OE1	1:B:204:ALA:HB1	0.45	2.11	96	1
1:B:189:LEU:HD11	1:B:193:ASN:HD22	0.45	1.71	97	1
1:A:98:GLU:OE1	1:A:98:GLU:C	0.45	2.60	97	10
1:A:18:ARG:CZ	1:A:21:ASN:ND2	0.45	2.80	54	1
1:A:171:THR:O	1:A:175:GLU:OE1	0.45	2.35	54	2
1:A:32:PHE:CE1	1:A:145:TYR:CG	0.45	3.04	57	1
1:A:203:LYS:CE	1:B:30:LYS:NZ	0.45	2.79	84	1
1:B:17:PRO:O	1:B:18:ARG:NH2	0.45	2.49	92	1
1:A:35:GLU:OE2	1:B:204:ALA:O	0.45	2.34	96	1
1:B:44:SER:CB	1:B:131:LYS:HZ2	0.45	2.24	77	4
1:A:179:GLN:H	1:A:179:GLN:NE2	0.45	2.09	45	2
1:A:213:GLU:O	1:A:216:THR:OG1	0.45	2.31	54	6
1:A:75:GLU:OE1	1:A:75:GLU:C	0.45	2.60	70	2
1:B:28:GLU:OE1	1:B:29:GLU:OE1	0.45	2.34	66	1
1:B:140:LYS:N	1:B:143:ARG:HH21	0.45	2.09	97	2
1:A:4:GLN:O	1:A:4:GLN:OE1	0.45	2.34	42	10
1:A:15:ILE:HD11	1:A:51:ASP:HB3	0.45	1.88	94	14
1:B:5:ASN:CG	1:B:7:GLN:OE1	0.45	2.59	61	4
1:A:202:LEU:HD21	1:A:218:CYS:SG	0.45	2.52	13	3
1:A:69:LEU:HD21	1:A:138:LEU:CD2	0.45	2.42	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:ILE:HG22	1:A:150:ILE:O	0.45	2.11	18	1
1:A:7:GLN:O	1:A:7:GLN:OE1	0.45	2.35	22	4
1:A:7:GLN:OE1	1:A:9:GLN:CD	0.45	2.59	48	4
1:B:69:LEU:HD21	1:B:138:LEU:CD2	0.45	2.42	48	4
1:B:211:LEU:HD12	1:B:212:GLU:H	0.45	1.71	89	3
1:A:145:TYR:CD2	1:A:145:TYR:C	0.45	2.91	37	1
1:A:143:ARG:HH22	1:A:170:LYS:HZ1	0.45	1.51	43	1
1:B:139:ASN:ND2	1:B:143:ARG:CZ	0.45	2.80	52	1
1:A:28:GLU:OE1	1:A:29:GLU:CD	0.45	2.60	68	1
1:B:103:ASP:OD1	1:B:108:THR:OG1	0.45	2.33	46	12
1:B:33:SER:OG	1:B:35:GLU:OE1	0.45	2.35	98	2
1:B:32:PHE:CE2	1:B:145:TYR:CE1	0.45	3.05	98	1
1:A:103:ASP:OD1	1:A:108:THR:OG1	0.45	2.34	50	11
1:B:32:PHE:CE2	1:B:145:TYR:O	0.45	2.70	38	1
1:B:67:GLN:CD	1:B:67:GLN:O	0.45	2.60	48	1
1:B:37:ILE:HD13	1:B:139:ASN:ND2	0.45	2.27	51	1
1:A:2:ILE:CD1	1:A:2:ILE:N	0.45	2.80	59	1
1:A:140:LYS:HZ3	1:A:143:ARG:NH2	0.45	2.08	64	1
1:A:141:ILE:CG2	1:A:145:TYR:CE2	0.45	3.00	64	1
1:B:150:ILE:HG13	1:B:151:LEU:N	0.45	2.26	9	1
1:B:210:THR:OG1	1:B:213:GLU:OE2	0.45	2.34	13	4
1:A:68:MET:CE	1:A:144:MET:SD	0.45	3.05	47	1
1:A:163:ASP:OD1	1:A:167:ARG:NH1	0.45	2.50	56	1
1:A:61:GLY:HA2	1:A:158:LYS:NZ	0.45	2.27	92	1
1:A:12:HIS:NE2	1:A:50:GLN:NE2	0.44	2.65	7	1
1:B:98:GLU:CD	1:B:98:GLU:O	0.44	2.59	12	7
1:B:195:ASN:CG	1:B:197:ASP:OD1	0.44	2.60	13	6
1:A:184:TRP:CZ2	1:A:189:LEU:HD23	0.44	2.46	47	3
1:A:184:TRP:CE3	1:A:185:MET:SD	0.44	3.11	59	4
1:B:155:GLN:NE2	1:B:195:ASN:CG	0.44	2.76	24	4
1:B:75:GLU:N	1:B:75:GLU:OE1	0.44	2.50	34	3
1:A:44:SER:HB2	1:A:131:LYS:HZ2	0.44	1.72	69	3
1:B:6:LEU:O	1:B:6:LEU:CD1	0.44	2.64	70	2
1:A:21:ASN:ND2	1:A:25:LYS:HZ2	0.44	2.10	92	1
1:A:132:ARG:NH2	1:A:133:TRP:HE1	0.44	2.10	96	1
1:A:96:MET:SD	1:A:96:MET:C	0.44	3.01	46	5
1:B:110:THR:OG1	1:B:113:GLU:OE1	0.44	2.31	59	3
1:A:26:VAL:HG13	1:A:39:MET:SD	0.44	2.52	52	6
1:A:100:ARG:HG3	1:A:102:SER:H	0.44	1.72	57	2
1:B:63:GLN:H	1:B:63:GLN:CD	0.44	2.19	72	1
1:B:63:GLN:CD	1:B:63:GLN:C	0.44	2.84	89	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:ASP:OD1	1:A:152:ASP:C	0.44	2.60	90	1
1:B:17:PRO:CB	1:B:18:ARG:HH21	0.44	2.25	92	2
1:A:44:SER:CB	1:A:131:LYS:NZ	0.44	2.81	25	15
1:B:150:ILE:HD12	1:B:185:MET:HG3	0.44	1.89	37	1
1:A:86:VAL:HG13	1:A:97:ARG:HH21	0.44	1.70	49	2
1:B:167:ARG:CZ	1:B:171:THR:OG1	0.44	2.65	51	1
1:A:184:TRP:CZ3	1:A:189:LEU:HD23	0.44	2.47	68	1
1:A:95:GLN:OE1	1:A:96:MET:C	0.44	2.61	2	7
1:A:121:ASN:OD1	1:A:121:ASN:C	0.44	2.60	17	10
1:B:12:HIS:HE2	1:B:48:THR:CG2	0.44	2.26	4	2
1:A:35:GLU:OE2	1:A:39:MET:HE3	0.44	2.12	84	3
1:A:18:ARG:NH2	1:A:21:ASN:HD22	0.44	2.09	13	2
1:B:151:LEU:HD12	1:B:151:LEU:N	0.44	2.27	15	3
1:B:62:HIS:CD2	1:B:65:ALA:CB	0.44	3.01	78	7
1:A:12:HIS:CD2	1:A:111:LEU:HD21	0.44	2.47	99	6
1:B:159:GLU:OE2	1:B:163:ASP:CG	0.44	2.61	52	2
1:A:50:GLN:CD	1:A:50:GLN:C	0.44	2.86	65	19
1:A:76:GLU:OE1	1:A:76:GLU:C	0.44	2.61	2	8
1:A:76:GLU:OE1	1:A:76:GLU:O	0.44	2.35	78	11
1:B:219:GLN:O	1:B:219:GLN:CG	0.44	2.65	74	6
1:A:68:MET:O	1:A:72:THR:HG23	0.44	2.12	88	5
1:B:4:GLN:NE2	1:B:10:MET:SD	0.44	2.90	46	1
1:B:113:GLU:OE1	1:B:113:GLU:O	0.44	2.36	64	1
1:A:2:ILE:C	1:A:2:ILE:CD1	0.44	2.83	68	1
1:A:176:GLN:N	1:A:176:GLN:OE1	0.44	2.51	88	1
1:B:94:GLY:C	1:B:95:GLN:OE1	0.44	2.61	94	1
1:A:96:MET:SD	1:A:120:HIS:CD2	0.44	3.10	38	4
1:A:97:ARG:HE	1:A:97:ARG:N	0.44	2.07	32	2
1:A:67:GLN:O	1:A:71:GLU:OE2	0.44	2.35	88	2
1:A:75:GLU:OE2	1:A:79:GLU:OE2	0.44	2.36	99	2
1:B:97:ARG:HH21	1:B:100:ARG:NH2	0.44	2.11	62	1
1:A:29:GLU:CD	1:B:204:ALA:HA	0.44	2.38	90	1
1:B:124:ILE:N	1:B:124:ILE:CD1	0.44	2.81	9	5
1:A:42:ALA:O	1:A:45:GLU:OE1	0.44	2.36	11	1
1:A:32:PHE:CE1	1:A:145:TYR:CD2	0.44	3.06	47	1
1:A:118:MET:CE	1:A:127:GLY:H	0.44	2.25	72	1
1:A:118:MET:HE1	1:A:128:GLU:OE2	0.44	2.11	88	1
1:B:154:ARG:NH2	1:B:155:GLN:O	0.44	2.50	97	1
1:A:2:ILE:H	1:A:2:ILE:CD1	0.44	2.26	45	9
1:B:91:ILE:HG23	1:B:91:ILE:O	0.44	2.13	19	4
1:B:80:TRP:CE2	1:B:84:HIS:CD2	0.44	3.05	94	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:179:GLN:CD	1:A:179:GLN:N	0.44	2.76	45	2
1:A:179:GLN:O	1:A:183:ASN:OD1	0.44	2.35	55	1
1:B:132:ARG:HH21	1:B:133:TRP:HE1	0.44	1.54	70	1
1:A:162:ARG:NH2	1:A:215:MET:HE3	0.44	2.28	71	1
1:A:144:MET:O	1:A:145:TYR:CE1	0.44	2.70	78	1
1:A:91:ILE:HD12	1:A:97:ARG:CZ	0.44	2.43	87	1
1:B:216:THR:O	1:B:219:GLN:CD	0.44	2.61	24	2
1:B:150:ILE:CD1	1:B:150:ILE:H	0.44	2.23	39	1
1:B:95:GLN:OE1	1:B:96:MET:C	0.44	2.61	68	5
1:B:150:ILE:CG2	1:B:185:MET:SD	0.44	3.06	78	1
1:A:7:GLN:HB3	1:A:9:GLN:NE2	0.44	2.27	89	1
1:A:209:ALA:HB3	1:A:214:MET:HE2	0.43	1.89	24	10
1:A:203:LYS:NZ	1:B:34:PRO:HG3	0.43	2.28	10	1
1:B:68:MET:O	1:B:72:THR:HG23	0.43	2.13	12	4
1:B:26:VAL:HG13	1:B:39:MET:SD	0.43	2.53	68	5
1:B:97:ARG:NH2	1:B:113:GLU:OE2	0.43	2.51	66	1
1:A:203:LYS:CB	1:A:203:LYS:NZ	0.43	2.80	68	1
1:A:219:GLN:OE1	1:A:219:GLN:O	0.43	2.36	20	10
1:B:123:PRO:C	1:B:124:ILE:HD12	0.43	2.38	9	5
1:A:4:GLN:O	1:A:4:GLN:CD	0.43	2.61	27	3
1:A:76:GLU:N	1:A:76:GLU:OE1	0.43	2.52	84	3
1:B:133:TRP:CD1	1:B:133:TRP:N	0.43	2.86	62	7
1:A:18:ARG:NH2	1:A:22:ALA:N	0.43	2.66	13	2
1:B:78:ALA:O	1:B:81:ASP:OD2	0.43	2.37	51	5
1:B:76:GLU:CD	1:B:133:TRP:CE2	0.43	2.96	47	1
1:B:219:GLN:O	1:B:219:GLN:CD	0.43	2.61	49	2
1:B:87:HIS:H	1:B:97:ARG:NH2	0.43	2.10	74	2
1:A:145:TYR:CD1	1:A:145:TYR:C	0.43	2.96	9	2
1:B:202:LEU:HD21	1:B:218:CYS:SG	0.43	2.53	74	4
1:A:145:TYR:C	1:A:145:TYR:CD2	0.43	2.95	99	2
1:B:100:ARG:NE	1:B:100:ARG:CA	0.43	2.82	52	3
1:A:185:MET:SD	1:A:185:MET:N	0.43	2.91	69	3
1:B:32:PHE:CD2	1:B:145:TYR:CD2	0.43	3.06	41	1
1:B:162:ARG:NE	1:B:163:ASP:OD1	0.43	2.52	60	2
1:A:7:GLN:O	1:A:7:GLN:HG2	0.43	2.14	53	2
1:B:76:GLU:O	1:B:76:GLU:OE1	0.43	2.35	90	1
1:A:61:GLY:CA	1:A:158:LYS:NZ	0.43	2.81	92	1
1:B:189:LEU:CD1	1:B:193:ASN:HD22	0.43	2.26	97	1
1:B:86:VAL:CG1	1:B:100:ARG:HE	0.43	2.26	1	1
1:A:139:ASN:HD21	1:A:167:ARG:CZ	0.43	2.27	3	1
1:A:80:TRP:CH2	1:A:84:HIS:CE1	0.43	3.05	15	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:98:GLU:CD	1:B:99:PRO:O	0.43	2.61	15	4
1:B:143:ARG:HH21	1:B:144:MET:CE	0.43	2.16	26	2
1:A:44:SER:OG	1:A:131:LYS:NZ	0.43	2.40	31	2
1:A:210:THR:OG1	1:A:213:GLU:OE2	0.43	2.30	84	3
1:B:152:ASP:OD1	1:B:152:ASP:C	0.43	2.61	73	2
1:B:10:MET:N	1:B:10:MET:SD	0.43	2.91	65	1
1:A:2:ILE:HD13	1:A:3:VAL:N	0.43	2.29	68	1
1:B:98:GLU:OE2	1:B:100:ARG:NH1	0.43	2.51	70	1
1:A:12:HIS:HE2	1:A:48:THR:CG2	0.43	2.26	6	3
1:B:91:ILE:O	1:B:91:ILE:HG23	0.43	2.13	4	3
1:A:28:GLU:CD	1:A:28:GLU:C	0.43	2.85	96	5
1:B:75:GLU:OE2	1:B:79:GLU:CD	0.43	2.61	21	4
1:B:120:HIS:ND1	1:B:122:PRO:O	0.43	2.47	23	4
1:A:121:ASN:O	1:A:121:ASN:OD1	0.43	2.36	90	3
1:B:153:ILE:HD11	1:B:167:ARG:CD	0.43	2.43	33	2
1:A:10:MET:N	1:A:10:MET:SD	0.43	2.92	86	3
1:B:18:ARG:HH21	1:B:21:ASN:ND2	0.43	2.11	54	1
1:B:143:ARG:HH22	1:B:157:PRO:HD3	0.43	1.73	63	1
1:B:15:ILE:HD13	1:B:55:MET:SD	0.43	2.53	67	1
1:A:16:SER:OG	1:A:19:THR:HG23	0.43	2.13	69	1
1:B:120:HIS:CE1	1:B:121:ASN:OD1	0.43	2.70	79	2
1:A:143:ARG:NE	1:A:143:ARG:HA	0.43	2.28	82	1
1:A:166:ASP:C	1:A:166:ASP:OD1	0.43	2.61	38	15
1:B:98:GLU:O	1:B:98:GLU:CD	0.43	2.61	66	2
1:B:98:GLU:CD	1:B:98:GLU:N	0.43	2.77	14	2
1:A:153:ILE:N	1:A:153:ILE:HD12	0.43	2.28	84	2
1:B:140:LYS:HZ2	1:B:143:ARG:HH21	0.43	1.56	24	1
1:B:30:LYS:N	1:B:30:LYS:CD	0.43	2.82	78	2
1:B:97:ARG:NE	1:B:100:ARG:HH12	0.43	2.10	35	1
1:B:143:ARG:CG	1:B:167:ARG:NH1	0.43	2.81	51	1
1:A:32:PHE:HB2	1:A:145:TYR:CD2	0.43	2.49	60	1
1:A:142:VAL:HG23	1:A:143:ARG:N	0.43	2.29	12	90
1:A:179:GLN:HE22	1:A:182:LYS:HZ1	0.43	1.54	34	1
1:B:163:ASP:OD1	1:B:166:ASP:OD2	0.43	2.36	98	2
1:B:213:GLU:OE1	1:B:213:GLU:CA	0.43	2.66	68	1
1:B:92:ALA:H	1:B:95:GLN:NE2	0.43	2.11	86	1
1:B:95:GLN:HG2	1:B:96:MET:N	0.43	2.29	7	3
1:A:4:GLN:CD	1:A:10:MET:HE1	0.43	2.39	9	1
1:B:144:MET:C	1:B:144:MET:SD	0.43	3.01	72	4
1:A:87:HIS:N	1:A:97:ARG:HH22	0.43	2.06	24	2
1:B:142:VAL:HG23	1:B:143:ARG:N	0.43	2.29	11	78

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:10:MET:HE3	1:B:119:THR:OG1	0.43	2.14	4	1
1:A:154:ARG:CD	1:A:155:GLN:O	0.43	2.67	20	2
1:B:7:GLN:CD	1:B:7:GLN:C	0.43	2.87	23	4
1:A:20:LEU:HD23	1:A:20:LEU:O	0.43	2.14	42	6
1:B:213:GLU:O	1:B:216:THR:OG1	0.43	2.31	96	7
1:A:171:THR:O	1:A:175:GLU:HG2	0.43	2.13	77	5
1:A:203:LYS:NZ	1:B:38:PRO:HG2	0.43	2.29	35	1
1:B:28:GLU:CD	1:B:28:GLU:C	0.43	2.87	38	3
1:B:12:HIS:CE1	1:B:50:GLN:OE1	0.43	2.71	49	2
1:A:75:GLU:OE2	1:A:79:GLU:CD	0.43	2.62	54	1
1:B:7:GLN:OE1	1:B:9:GLN:CD	0.43	2.62	67	1
1:B:143:ARG:NE	1:B:154:ARG:NH2	0.43	2.67	75	1
1:B:103:ASP:O	1:B:114:GLN:NE2	0.42	2.52	85	14
1:B:79:GLU:N	1:B:82:ARG:HH21	0.42	2.12	18	1
1:B:32:PHE:CE1	1:B:145:TYR:CD2	0.42	3.07	43	1
1:B:70:LYS:O	1:B:74:ASN:CG	0.42	2.62	54	1
1:A:192:GLN:OE1	1:A:193:ASN:OD1	0.42	2.37	87	1
1:B:79:GLU:OE1	1:B:79:GLU:N	0.42	2.51	93	1
1:A:175:GLU:OE2	1:A:176:GLN:N	0.42	2.50	97	1
1:A:167:ARG:HE	1:A:171:THR:HG23	0.42	1.73	3	2
1:B:80:TRP:CD2	1:B:84:HIS:CE1	0.42	3.08	52	1
1:B:189:LEU:O	1:B:189:LEU:HD13	0.42	2.13	97	2
1:B:79:GLU:O	1:B:79:GLU:OE1	0.42	2.37	54	1
1:A:42:ALA:CB	1:B:205:LEU:O	0.42	2.66	70	1
1:B:94:GLY:O	1:B:95:GLN:OE1	0.42	2.37	94	1
1:A:132:ARG:NH1	1:A:136:LEU:HD11	0.42	2.29	95	1
1:A:150:ILE:CD1	1:A:150:ILE:N	0.42	2.81	1	1
1:B:86:VAL:CG1	1:B:100:ARG:NH2	0.42	2.83	9	1
1:A:7:GLN:OE1	1:A:7:GLN:N	0.42	2.52	11	1
1:B:67:GLN:O	1:B:67:GLN:NE2	0.42	2.51	23	3
1:A:76:GLU:N	1:A:76:GLU:CD	0.42	2.76	29	1
1:B:121:ASN:OD1	1:B:121:ASN:C	0.42	2.62	55	3
1:A:57:ASN:ND2	1:A:57:ASN:C	0.42	2.77	97	1
1:B:114:GLN:OE1	1:B:114:GLN:CA	0.42	2.68	6	13
1:A:213:GLU:OE1	1:A:213:GLU:CA	0.42	2.66	39	2
1:A:98:GLU:CD	1:A:98:GLU:N	0.42	2.76	77	3
1:B:163:ASP:OD1	1:B:167:ARG:CZ	0.42	2.68	66	2
1:A:175:GLU:OE1	1:A:177:ALA:N	0.42	2.52	67	1
1:A:86:VAL:CG2	1:A:97:ARG:NH2	0.42	2.82	69	1
1:A:213:GLU:OE1	1:A:213:GLU:C	0.42	2.62	37	2
1:B:44:SER:CB	1:B:131:LYS:NZ	0.42	2.83	2	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:GLN:CD	1:A:63:GLN:C	0.42	2.86	86	3
1:A:203:LYS:NZ	1:B:38:PRO:CD	0.42	2.82	35	1
1:B:184:TRP:CZ3	1:B:189:LEU:HD23	0.42	2.50	50	1
1:B:81:ASP:OD2	1:B:82:ARG:NH1	0.42	2.52	93	1
1:A:95:GLN:OE1	1:A:96:MET:N	0.42	2.53	37	4
1:B:179:GLN:O	1:B:183:ASN:OD1	0.42	2.37	7	3
1:B:7:GLN:HB3	1:B:9:GLN:NE2	0.42	2.30	89	1
1:A:97:ARG:HE	1:A:100:ARG:NH1	0.42	2.12	92	1
1:B:195:ASN:ND2	1:B:197:ASP:CG	0.42	2.77	49	4
1:A:145:TYR:CD1	1:A:145:TYR:N	0.42	2.86	25	1
1:B:71:GLU:O	1:B:75:GLU:OE2	0.42	2.37	79	3
1:A:25:LYS:HZ3	1:A:25:LYS:CB	0.42	2.28	37	1
1:A:150:ILE:HD11	1:A:168:PHE:CZ	0.42	2.50	55	1
1:A:44:SER:OG	1:A:55:MET:SD	0.42	2.75	70	2
1:A:91:ILE:HD13	1:A:91:ILE:N	0.42	2.29	67	1
1:A:96:MET:CE	1:A:120:HIS:ND1	0.42	2.83	70	1
1:B:13:GLN:OE1	1:B:14:ALA:O	0.42	2.37	95	1
1:A:150:ILE:HD11	1:A:185:MET:SD	0.42	2.55	3	1
1:B:15:ILE:O	1:B:15:ILE:CD1	0.42	2.68	58	4
1:B:155:GLN:NE2	1:B:195:ASN:OD1	0.42	2.52	24	1
1:B:75:GLU:CD	1:B:75:GLU:O	0.42	2.61	55	2
1:B:143:ARG:HG3	1:B:167:ARG:NH1	0.42	2.30	51	1
1:A:18:ARG:HE	1:A:18:ARG:N	0.42	2.10	53	1
1:B:71:GLU:CD	1:B:71:GLU:C	0.42	2.88	60	2
1:B:97:ARG:HE	1:B:97:ARG:N	0.42	2.08	88	1
1:B:179:GLN:OE1	1:B:179:GLN:N	0.42	2.50	2	1
1:B:143:ARG:NH1	1:B:144:MET:SD	0.42	2.93	39	1
1:B:75:GLU:OE1	1:B:75:GLU:C	0.42	2.63	53	3
1:B:143:ARG:HE	1:B:154:ARG:NH2	0.42	2.13	75	1
1:A:112:GLN:NE2	1:A:112:GLN:H	0.42	2.12	88	1
1:B:79:GLU:CD	1:B:79:GLU:C	0.42	2.87	99	1
1:B:75:GLU:O	1:B:75:GLU:OE1	0.42	2.38	24	1
1:B:71:GLU:C	1:B:71:GLU:CD	0.42	2.87	46	1
1:B:12:HIS:C	1:B:13:GLN:OE1	0.42	2.63	54	1
1:B:70:LYS:O	1:B:74:ASN:OD1	0.42	2.37	54	1
1:B:139:ASN:O	1:B:143:ARG:HG2	0.42	2.15	70	1
1:B:219:GLN:CD	1:B:219:GLN:C	0.42	2.88	93	1
1:B:167:ARG:NE	1:B:167:ARG:CA	0.41	2.83	8	1
1:B:71:GLU:CD	1:B:71:GLU:O	0.41	2.64	46	1
1:A:80:TRP:CD1	1:A:104:ILE:CD1	0.41	3.04	52	1
1:A:177:ALA:HB3	1:A:182:LYS:NZ	0.41	2.31	99	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:5:ASN:OD1	1:B:9:GLN:O	0.41	2.38	68	1
1:A:41:SER:OG	1:B:203:LYS:C	0.41	2.62	70	1
1:B:162:ARG:HH21	1:B:215:MET:CE	0.41	2.28	95	1
1:A:112:GLN:N	1:A:112:GLN:CD	0.41	2.78	100	1
1:A:21:ASN:CG	1:A:25:LYS:HZ3	0.41	2.21	12	1
1:B:87:HIS:NE2	1:B:97:ARG:NH1	0.41	2.68	46	1
1:B:197:ASP:O	1:B:197:ASP:OD1	0.41	2.37	68	1
1:A:66:MET:HE1	1:A:67:GLN:NE2	0.41	2.30	69	1
1:A:182:LYS:HB2	1:A:182:LYS:HZ2	0.41	1.75	73	1
1:B:96:MET:CE	1:B:120:HIS:CE1	0.41	3.03	89	1
1:A:20:LEU:HD12	1:A:55:MET:SD	0.41	2.54	92	1
1:B:18:ARG:NH1	1:B:22:ALA:HB2	0.41	2.30	99	1
1:B:193:ASN:OD1	1:B:193:ASN:C	0.41	2.64	89	3
1:B:4:GLN:CD	1:B:4:GLN:C	0.41	2.88	36	2
1:B:139:ASN:CG	1:B:143:ARG:CZ	0.41	2.93	52	1
1:A:121:ASN:OD1	1:A:121:ASN:O	0.41	2.37	95	2
1:A:173:ARG:NH2	1:A:182:LYS:HZ2	0.41	2.12	69	1
1:A:132:ARG:NH2	1:A:133:TRP:NE1	0.41	2.69	96	1
1:B:167:ARG:HH11	1:B:171:THR:HG22	0.41	1.75	2	1
1:B:32:PHE:CD2	1:B:145:TYR:CE1	0.41	3.08	14	1
1:B:63:GLN:OE1	1:B:64:ALA:N	0.41	2.47	30	1
1:B:75:GLU:OE1	1:B:75:GLU:CA	0.41	2.69	79	3
1:A:150:ILE:HG23	1:A:171:THR:OG1	0.41	2.16	64	1
1:B:67:GLN:O	1:B:67:GLN:CD	0.41	2.64	23	1
1:A:186:THR:CG2	1:A:187:GLU:OE1	0.41	2.69	49	1
1:B:154:ARG:HE	1:B:154:ARG:C	0.41	2.24	64	1
1:A:195:ASN:CG	1:A:197:ASP:OD1	0.41	2.63	70	2
1:A:30:LYS:NZ	1:A:35:GLU:OE1	0.41	2.40	82	1
1:B:155:GLN:CD	1:B:195:ASN:HD22	0.41	2.24	87	1
1:A:203:LYS:NZ	1:A:203:LYS:CB	0.41	2.84	98	1
1:B:95:GLN:N	1:B:95:GLN:CD	0.41	2.78	100	1
1:B:56:LEU:HD11	1:B:69:LEU:HD13	0.41	1.92	17	6
1:B:34:PRO:HG2	1:B:152:ASP:OD1	0.41	2.15	3	1
1:A:12:HIS:C	1:A:13:GLN:OE1	0.41	2.63	99	2
1:B:85:PRO:O	1:B:87:HIS:CE1	0.41	2.73	82	1
1:A:50:GLN:OE1	1:A:54:THR:OG1	0.41	2.39	11	1
1:B:155:GLN:OE1	1:B:159:GLU:O	0.41	2.38	24	1
1:A:150:ILE:HD13	1:A:175:GLU:OE1	0.41	2.16	33	1
1:A:150:ILE:HD13	1:A:150:ILE:N	0.41	2.16	40	1
1:A:100:ARG:CA	1:A:100:ARG:NE	0.41	2.84	64	1
1:B:211:LEU:O	1:B:211:LEU:HD23	0.41	2.15	87	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:95:GLN:O	1:B:96:MET:CE	0.41	2.69	78	1
1:A:21:ASN:CG	1:A:25:LYS:HZ2	0.41	2.23	92	1
1:B:12:HIS:CD2	1:B:48:THR:HG21	0.41	2.51	4	3
1:A:96:MET:HE2	1:A:117:TRP:CD1	0.41	2.51	6	1
1:A:2:ILE:HD12	1:A:118:MET:SD	0.41	2.56	93	2
1:B:91:ILE:CD1	1:B:97:ARG:HH21	0.41	2.28	36	1
1:B:32:PHE:CZ	1:B:145:TYR:CE2	0.41	3.09	43	1
1:B:143:ARG:HG3	1:B:167:ARG:HH12	0.41	1.76	51	1
1:A:139:ASN:OD1	1:A:143:ARG:CD	0.41	2.69	60	1
1:B:162:ARG:CZ	1:B:163:ASP:OD1	0.41	2.68	60	1
1:B:20:LEU:HD12	1:B:55:MET:SD	0.41	2.56	65	3
1:B:145:TYR:O	1:B:145:TYR:CD2	0.41	2.74	69	1
1:B:195:ASN:CG	1:B:198:CYS:SG	0.41	3.04	72	1
1:A:12:HIS:CD2	1:A:12:HIS:N	0.41	2.89	76	2
1:B:179:GLN:CD	1:B:179:GLN:N	0.41	2.77	82	1
1:B:4:GLN:OE1	1:B:4:GLN:N	0.41	2.48	86	1
1:A:79:GLU:OE1	1:A:82:ARG:NH2	0.41	2.49	88	1
1:A:129:ILE:O	1:A:133:TRP:CD1	0.41	2.74	93	1
1:B:96:MET:HE1	1:B:117:TRP:CE2	0.41	2.51	91	3
1:B:94:GLY:O	1:B:96:MET:HE1	0.41	2.16	37	1
1:B:152:ASP:O	1:B:152:ASP:CG	0.41	2.63	38	3
1:B:145:TYR:CD1	1:B:145:TYR:O	0.41	2.73	41	1
1:B:133:TRP:N	1:B:133:TRP:CD1	0.41	2.87	47	1
1:B:75:GLU:C	1:B:75:GLU:CD	0.41	2.89	73	2
1:A:76:GLU:HG2	1:A:133:TRP:CD1	0.41	2.50	93	2
1:A:173:ARG:HH21	1:A:182:LYS:NZ	0.41	2.13	87	1
1:B:67:GLN:HG3	1:B:68:MET:N	0.40	2.31	30	1
1:A:133:TRP:N	1:A:133:TRP:CD1	0.40	2.89	78	3
1:B:97:ARG:CD	1:B:97:ARG:N	0.40	2.84	99	2
1:B:63:GLN:HG3	1:B:64:ALA:N	0.40	2.30	62	1
1:B:86:VAL:HG13	1:B:100:ARG:NH1	0.40	2.31	74	1
1:A:12:HIS:CE1	1:A:112:GLN:NE2	0.40	2.89	100	1
1:A:77:ALA:O	1:A:81:ASP:CG	0.40	2.65	8	1
1:A:77:ALA:O	1:A:81:ASP:OD2	0.40	2.39	8	3
1:B:98:GLU:CD	1:B:98:GLU:C	0.40	2.89	15	2
1:A:50:GLN:OE1	1:A:111:LEU:HD13	0.40	2.15	93	3
1:B:81:ASP:OD2	1:B:100:ARG:CZ	0.40	2.69	20	1
1:B:87:HIS:NE2	1:B:98:GLU:OE1	0.40	2.52	31	1
1:A:71:GLU:CD	1:A:71:GLU:C	0.40	2.88	54	1
1:A:29:GLU:OE1	1:A:30:LYS:NZ	0.40	2.55	67	1
1:B:199:LYS:CB	1:B:199:LYS:NZ	0.40	2.84	69	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:HIS:NE2	1:A:98:GLU:CG	0.40	2.84	74	1
1:B:35:GLU:OE2	1:B:39:MET:HE3	0.40	2.17	85	1
1:A:32:PHE:CD2	1:A:145:TYR:CE2	0.40	3.09	86	1
1:A:103:ASP:CG	1:A:109:SER:HG	0.40	2.23	90	1
1:A:172:LEU:CD1	1:A:185:MET:SD	0.40	3.10	26	1
1:A:167:ARG:O	1:A:167:ARG:NE	0.40	2.50	31	1
1:A:25:LYS:CB	1:A:25:LYS:NZ	0.40	2.84	37	1
1:B:87:HIS:N	1:B:97:ARG:HH22	0.40	2.14	37	1
1:A:166:ASP:CG	1:A:167:ARG:NH2	0.40	2.80	57	1
1:A:113:GLU:CD	1:A:117:TRP:CZ3	0.40	2.99	62	1
1:A:215:MET:SD	1:A:215:MET:C	0.40	3.04	63	1
1:A:192:GLN:HE21	1:A:193:ASN:ND2	0.40	2.14	70	1
1:B:112:GLN:CD	1:B:112:GLN:C	0.40	2.89	70	1
1:A:21:ASN:O	1:A:21:ASN:OD1	0.40	2.38	71	1
1:A:98:GLU:CD	1:A:100:ARG:HH11	0.40	2.25	74	1
1:B:75:GLU:C	1:B:75:GLU:OE1	0.40	2.65	78	1
1:A:35:GLU:OE2	1:B:204:ALA:CB	0.40	2.67	86	1
1:B:152:ASP:C	1:B:152:ASP:OD1	0.40	2.65	98	1
1:B:15:ILE:CG2	1:B:19:THR:OG1	0.40	2.70	11	2
1:A:189:LEU:CD2	1:A:193:ASN:ND2	0.40	2.83	12	1
1:B:162:ARG:CD	1:B:215:MET:SD	0.40	3.09	51	1
1:B:192:GLN:C	1:B:192:GLN:NE2	0.40	2.80	54	1
1:B:142:VAL:CG2	1:B:143:ARG:N	0.40	2.85	70	1
1:A:66:MET:SD	1:A:66:MET:C	0.40	3.04	93	2
1:A:12:HIS:CD2	1:A:48:THR:HG21	0.40	2.52	1	1
1:A:1:PRO:HB2	1:A:2:ILE:HD12	0.40	1.94	2	1
1:B:150:ILE:O	1:B:151:LEU:C	0.40	2.65	4	1
1:A:143:ARG:HH11	1:A:171:THR:HG22	0.40	1.77	8	1
1:A:203:LYS:NZ	1:B:34:PRO:CG	0.40	2.84	10	1
1:B:33:SER:O	1:B:36:VAL:HG12	0.40	2.17	28	1
1:A:181:VAL:CG1	1:A:185:MET:HE3	0.40	2.38	31	1
1:B:167:ARG:HH11	1:B:171:THR:CG2	0.40	2.29	82	1
1:A:150:ILE:O	1:A:152:ASP:N	0.40	2.55	88	1
1:A:173:ARG:HH22	1:A:182:LYS:NZ	0.40	2.14	94	1
1:A:121:ASN:C	1:A:121:ASN:OD1	0.40	2.64	96	1
1:A:76:GLU:OE2	1:A:80:TRP:CZ3	0.40	2.75	97	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	215/231 (93%)	211±1 (98±0%)	2±1 (1±0%)	2±1 (1±0%)	18	68
1	B	215/231 (93%)	211±1 (98±0%)	2±1 (1±0%)	2±1 (1±0%)	20	70
All	All	43000/46200 (93%)	42177 (98%)	493 (1%)	330 (1%)	18	68

All 8 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	31	ALA	100
1	B	31	ALA	100
1	A	150	ILE	47
1	B	150	ILE	30
1	B	145	TYR	28
1	A	145	TYR	23
1	B	151	LEU	1
1	A	151	LEU	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	184/194 (95%)	172±2 (94±1%)	12±2 (6±1%)	18	67
1	B	184/194 (95%)	172±3 (93±2%)	12±3 (7±2%)	17	65
All	All	36800/38800 (95%)	34409 (94%)	2391 (6%)	17	66

All 159 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	180	GLU	100
1	B	178	SER	100
1	B	180	GLU	100
1	A	178	SER	99
1	B	198	CYS	87
1	A	198	CYS	86
1	A	193	ASN	51
1	B	24	VAL	46
1	B	189	LEU	46
1	A	150	ILE	45
1	A	195	ASN	43
1	B	58	THR	42
1	B	195	ASN	41
1	B	96	MET	40
1	B	10	MET	38
1	A	10	MET	34
1	A	58	THR	34
1	B	15	ILE	33
1	A	96	MET	32
1	A	2	ILE	31
1	A	24	VAL	31
1	A	6	LEU	30
1	A	108	THR	30
1	A	159	GLU	30
1	B	193	ASN	29
1	A	192	GLN	28
1	B	159	GLU	28
1	B	76	GLU	25
1	A	7	GLN	25
1	A	100	ARG	24
1	A	4	GLN	24
1	A	15	ILE	24
1	B	150	ILE	24
1	A	136	LEU	23
1	B	4	GLN	22
1	A	175	GLU	21
1	B	145	TYR	20
1	B	68	MET	19
1	B	100	ARG	19
1	A	189	LEU	19
1	B	53	ASN	19
1	B	91	ILE	19
1	B	6	LEU	19

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Mol	Chain	Res	Type	Models (Total)
1	B	67	GLN	18
1	A	76	GLU	18
1	A	213	GLU	18
1	B	213	GLU	18
1	A	74	ASN	17
1	B	63	GLN	17
1	B	192	GLN	17
1	A	145	TYR	17
1	B	155	GLN	17
1	B	175	GLU	16
1	B	143	ARG	15
1	B	108	THR	15
1	A	120	HIS	14
1	A	219	GLN	14
1	B	114	GLN	14
1	B	170	LYS	14
1	B	7	GLN	14
1	A	25	LYS	13
1	B	75	GLU	13
1	A	68	MET	12
1	B	167	ARG	12
1	B	97	ARG	12
1	B	191	VAL	11
1	A	176	GLN	10
1	A	167	ARG	10
1	B	83	LEU	10
1	B	107	THR	10
1	A	39	MET	9
1	B	81	ASP	9
1	B	2	ILE	9
1	A	158	LYS	9
1	A	82	ARG	8
1	B	25	LYS	7
1	B	179	GLN	7
1	A	67	GLN	7
1	A	170	LYS	7
1	B	98	GLU	7
1	B	203	LYS	7
1	B	95	GLN	7
1	B	163	ASP	7
1	B	199	LYS	7
1	B	39	MET	7

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Mol	Chain	Res	Type	Models (Total)
1	A	203	LYS	7
1	A	139	ASN	6
1	B	176	GLN	6
1	A	113	GLU	6
1	B	74	ASN	6
1	A	18	ARG	6
1	A	12	HIS	6
1	A	153	ILE	5
1	B	154	ARG	5
1	A	97	ARG	5
1	A	107	THR	5
1	B	185	MET	5
1	A	132	ARG	4
1	B	79	GLU	4
1	A	9	GLN	4
1	A	79	GLU	4
1	A	66	MET	4
1	B	110	THR	4
1	B	219	GLN	4
1	B	18	ARG	4
1	A	21	ASN	4
1	B	136	LEU	4
1	B	205	LEU	4
1	B	66	MET	3
1	A	179	GLN	3
1	B	197	ASP	3
1	B	140	LYS	3
1	A	152	ASP	3
1	B	50	GLN	3
1	A	119	THR	3
1	A	173	ARG	3
1	B	211	LEU	3
1	A	71	GLU	3
1	A	112	GLN	3
1	B	184	TRP	3
1	A	91	ILE	3
1	A	154	ARG	2
1	B	158	LYS	2
1	A	5	ASN	2
1	A	57	ASN	2
1	B	19	THR	2
1	B	113	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	B	215	MET	2
1	A	199	LYS	2
1	B	70	LYS	2
1	B	166	ASP	2
1	B	173	ARG	2
1	A	13	GLN	2
1	A	83	LEU	2
1	A	143	ARG	2
1	A	191	VAL	2
1	B	13	GLN	2
1	B	82	ARG	2
1	B	119	THR	2
1	B	153	ILE	2
1	B	138	LEU	2
1	B	121	ASN	2
1	B	162	ARG	2
1	B	152	ASP	1
1	A	81	ASP	1
1	A	84	HIS	1
1	B	218	CYS	1
1	B	144	MET	1
1	A	19	THR	1
1	A	162	ARG	1
1	A	16	SER	1
1	B	16	SER	1
1	B	62	HIS	1
1	B	30	LYS	1
1	A	62	HIS	1
1	B	20	LEU	1
1	A	70	LYS	1
1	B	132	ARG	1
1	A	185	MET	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 [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 15% for the well-defined parts and 15% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	919
Number of shifts mapped to atoms	875
Number of unparsed shifts	0
Number of shifts with mapping errors	44
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 44 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	222	GLY	H	8.564	0.020	1
1	A	222	GLY	C	174.142	0.200	1
1	A	222	GLY	CA	44.634	0.061	1
1	A	222	GLY	N	115.571	0.200	1
1	A	223	GLY	H	7.914	0.020	1
1	A	223	GLY	C	172.071	0.200	1
1	A	223	GLY	CA	44.124	0.017	1
1	A	223	GLY	N	108.695	0.200	1
1	A	224	PRO	C	177.859	0.200	1
1	A	224	PRO	CA	63.23	0.200	1
1	A	224	PRO	CB	31.122	0.200	1
1	A	225	GLY	H	8.415	0.020	1
1	A	225	GLY	C	174.067	0.200	1
1	A	225	GLY	CA	44.876	0.046	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	225	GLY	N	109.29	0.200	1
1	A	226	HIS	H	8.049	0.020	1
1	A	226	HIS	CA	55.859	0.050	1
1	A	226	HIS	CB	28.879	0.200	1
1	A	226	HIS	N	119.896	0.001	1
1	A	227	LYS	H	8.119	0.020	1
1	A	227	LYS	C	175.898	0.200	1
1	A	227	LYS	CA	55.628	0.015	1
1	A	227	LYS	CB	31.893	0.052	1
1	A	227	LYS	N	123.533	0.001	1
1	A	228	ALA	H	8.147	0.020	1
1	A	228	ALA	C	177.383	0.200	1
1	A	228	ALA	CA	51.938	0.005	1
1	A	228	ALA	CB	18.4	0.011	1
1	A	228	ALA	N	125.611	0.200	1
1	A	229	ARG	H	8.166	0.020	1
1	A	229	ARG	C	175.894	0.200	1
1	A	229	ARG	CA	55.627	0.003	1
1	A	229	ARG	CB	29.898	0.005	1
1	A	229	ARG	N	121.107	0.200	1
1	A	230	VAL	H	8.09	0.020	1
1	A	230	VAL	C	175.019	0.200	1
1	A	230	VAL	CA	61.973	0.036	1
1	A	230	VAL	CB	31.729	0.005	1
1	A	230	VAL	N	123.017	0.200	1
1	A	231	LEU	H	7.756	0.020	1
1	A	231	LEU	C	182.069	0.200	1
1	A	231	LEU	CA	56.348	0.200	1
1	A	231	LEU	CB	42.383	0.200	1
1	A	231	LEU	N	131.803	0.200	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	200	0.09 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	173	1.36 ± 0.09	Should be checked
$^{13}\text{C}'$	190	-0.39 ± 0.10	None needed (< 0.5 ppm)
^{15}N	178	0.08 ± 0.24	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 15%, i.e. 875 atoms were assigned a chemical shift out of a possible 5948. 0 out of 62 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	709/2136 (33%)	169/866 (20%)	371/868 (43%)	169/402 (42%)
Sidechain	166/3460 (5%)	0/2258 (0%)	166/1072 (15%)	0/130 (0%)
Aromatic	0/352 (0%)	0/172 (0%)	0/150 (0%)	0/30 (0%)
Overall	875/5948 (15%)	169/3296 (5%)	537/2090 (26%)	169/562 (30%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 15%, i.e. 875 atoms were assigned a chemical shift out of a possible 6026. 0 out of 62 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	709/2172 (33%)	169/880 (19%)	371/884 (42%)	169/408 (41%)
Sidechain	166/3502 (5%)	0/2286 (0%)	166/1086 (15%)	0/130 (0%)
Aromatic	0/352 (0%)	0/172 (0%)	0/150 (0%)	0/30 (0%)
Overall	875/6026 (15%)	169/3338 (5%)	537/2120 (25%)	169/568 (30%)

7.1.4 Statistically unusual chemical shifts [i](#)

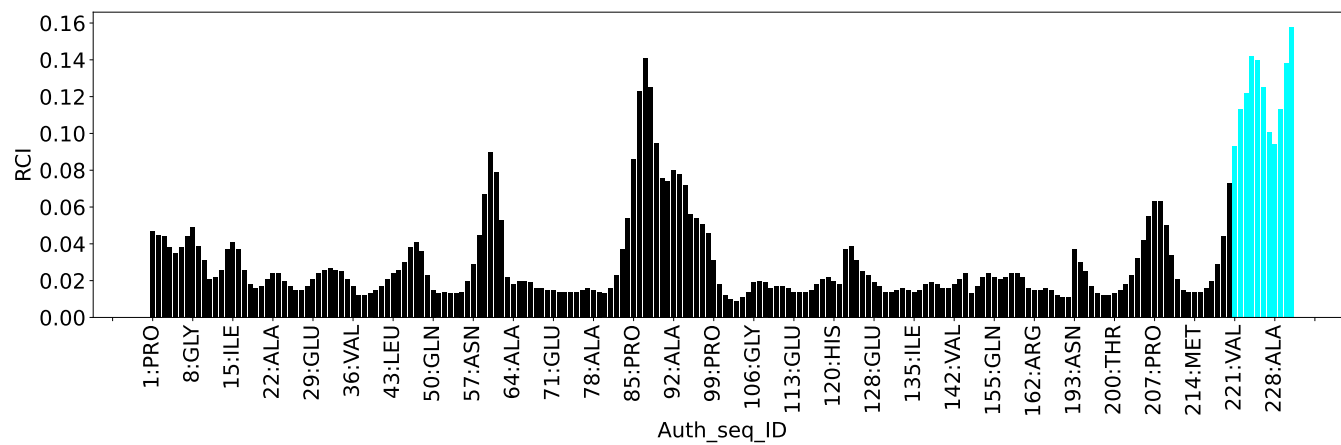
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	101	GLY	H	11.58	5.23 – 11.42	5.2

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

No restraints data found

9 Distance violation analysis ⓘ

No distance restraints data found

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found