



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 06:57 pm GMT

PDB ID : 1NCS
Title : NMR STUDY OF SWI5 ZINC FINGER DOMAIN 1
Authors : Dutnall, R.N.; Neuhaus, D.; Rhodes, D.
Deposited on : 1996-02-26

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

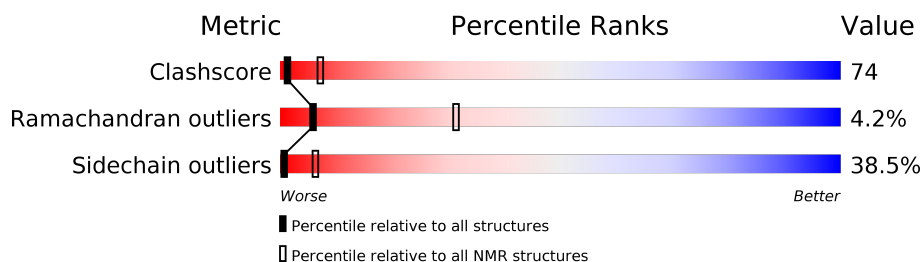
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	47	

2 Ensemble composition and analysis

This entry contains 46 models. Model 16 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:20-A:57 (38)	0.27	16

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 5 clusters and 7 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 797 atoms, of which 399 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TRANSCRIPTIONAL FACTOR SWI5.

Mol	Chain	Residues	Atoms						Trace
1	A	47	Total	C	H	N	O	S	0
			796	250	399	73	71	3	

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

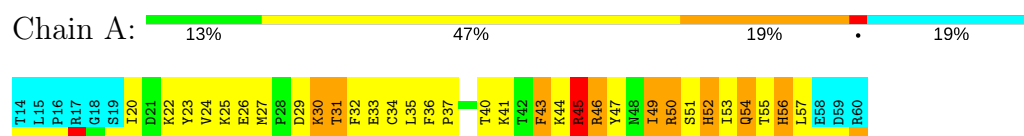
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5

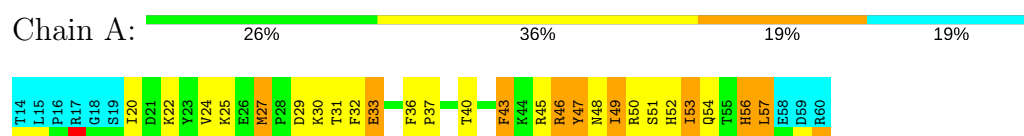


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

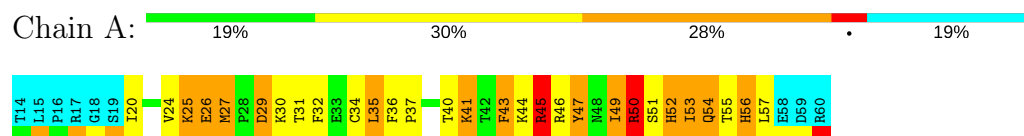
4.2.1 Score per residue for model 1

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



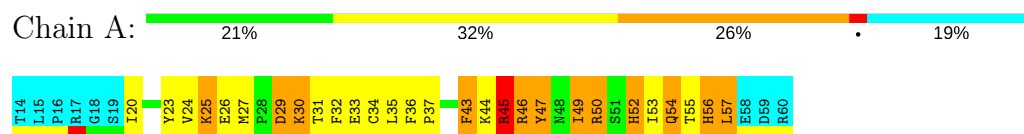
4.2.2 Score per residue for model 2

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



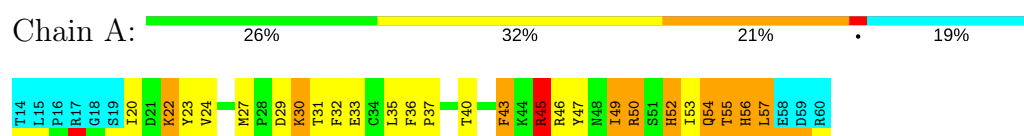
4.2.3 Score per residue for model 3

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



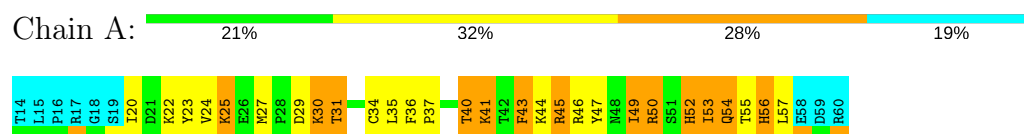
4.2.4 Score per residue for model 4

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



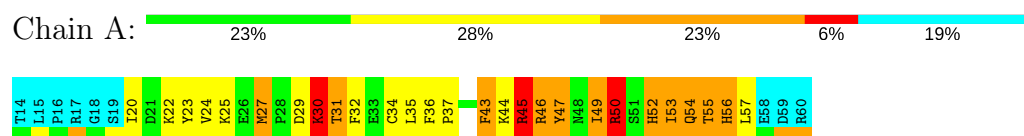
4.2.5 Score per residue for model 5

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



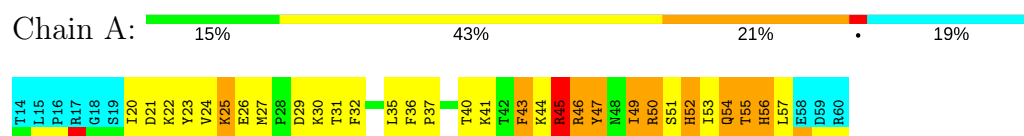
4.2.6 Score per residue for model 6

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



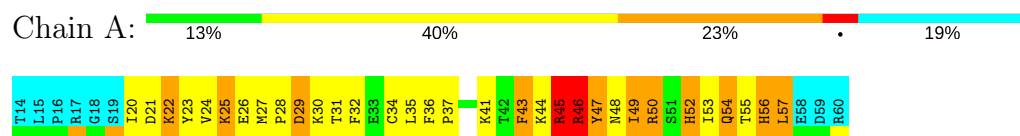
4.2.7 Score per residue for model 7

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



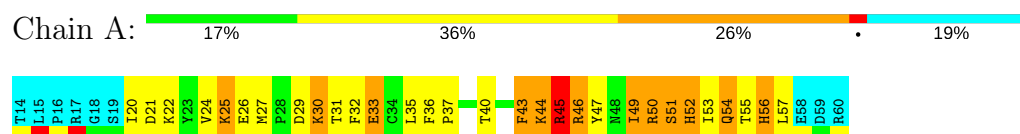
4.2.8 Score per residue for model 8

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



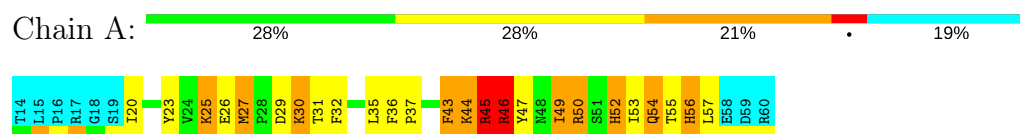
4.2.9 Score per residue for model 9

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



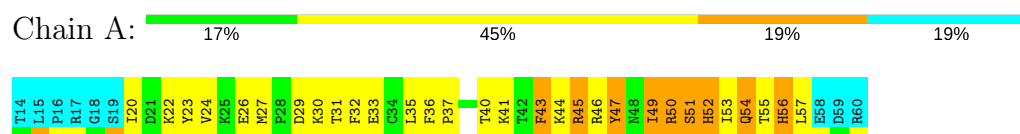
4.2.10 Score per residue for model 10

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



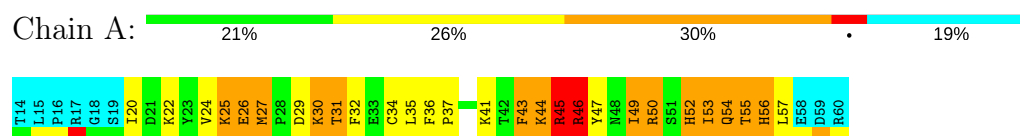
4.2.11 Score per residue for model 11

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



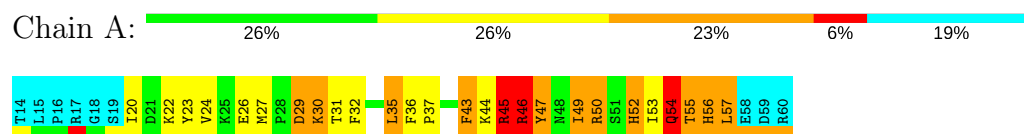
4.2.12 Score per residue for model 12

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



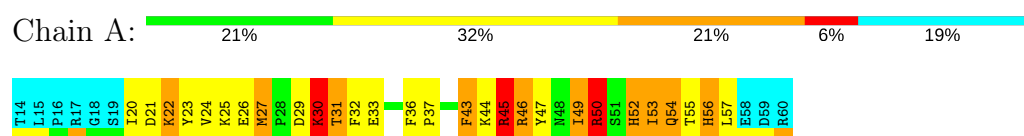
4.2.13 Score per residue for model 13

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



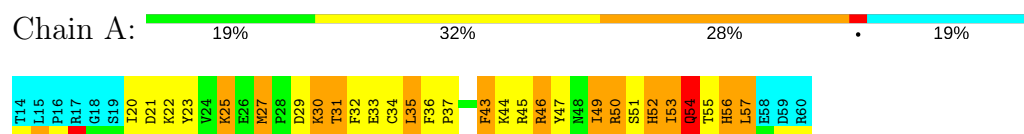
4.2.14 Score per residue for model 14

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



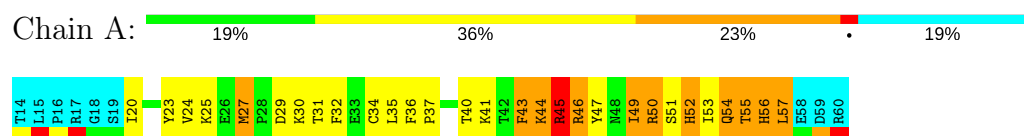
4.2.15 Score per residue for model 15

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



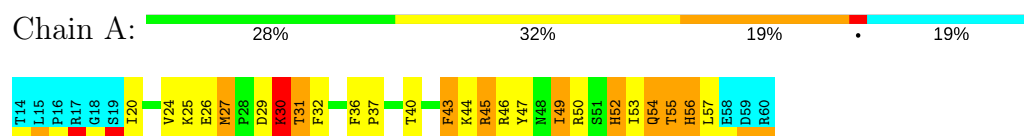
4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



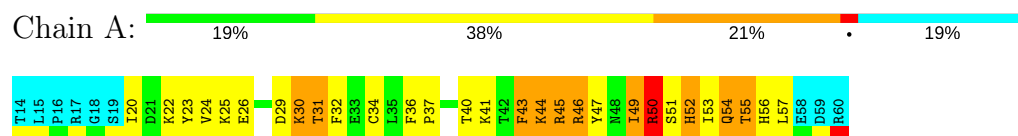
4.2.17 Score per residue for model 17

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



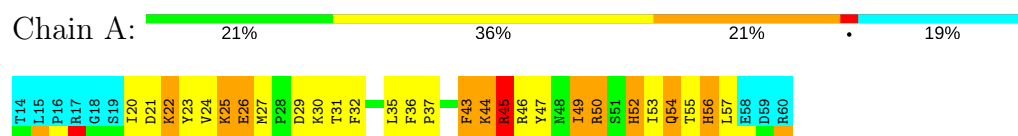
4.2.18 Score per residue for model 18

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



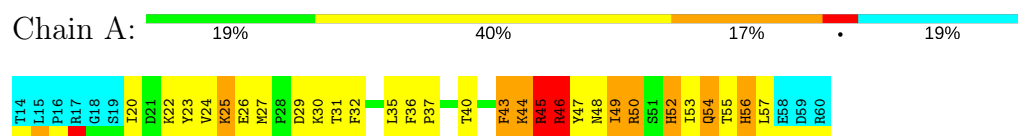
4.2.19 Score per residue for model 19

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



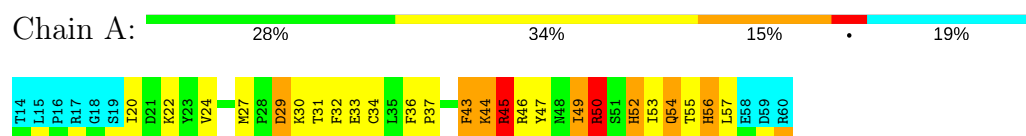
4.2.20 Score per residue for model 20

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



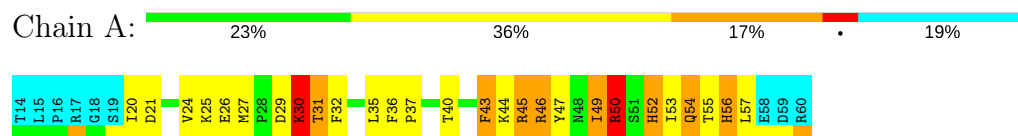
4.2.21 Score per residue for model 21

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



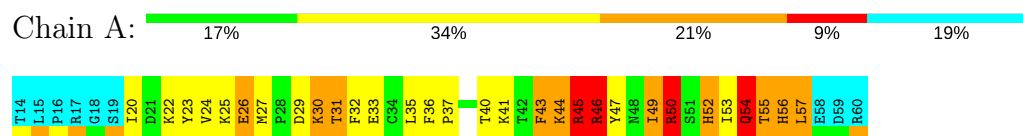
4.2.22 Score per residue for model 22

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



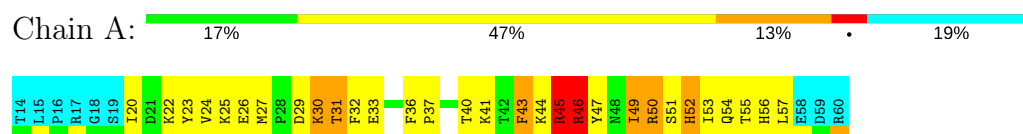
4.2.23 Score per residue for model 23

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



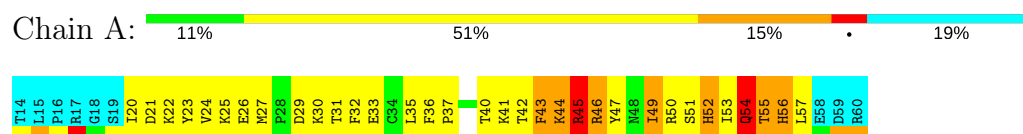
4.2.24 Score per residue for model 24

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



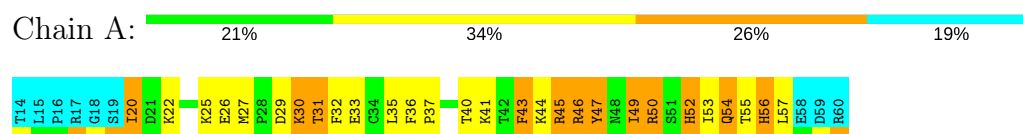
4.2.25 Score per residue for model 25

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



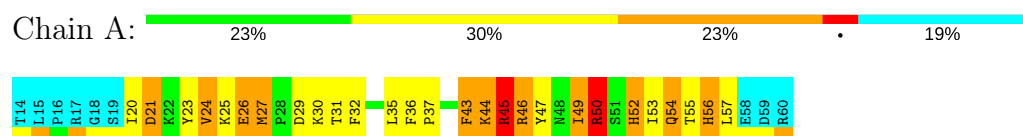
4.2.26 Score per residue for model 26

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



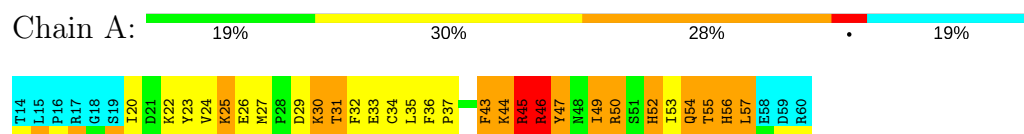
4.2.27 Score per residue for model 27

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



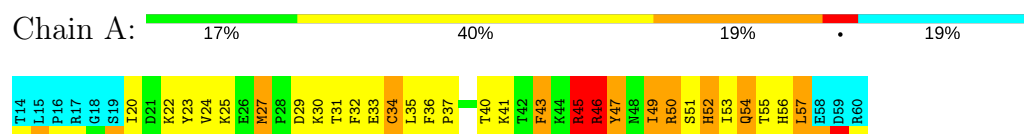
4.2.28 Score per residue for model 28

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



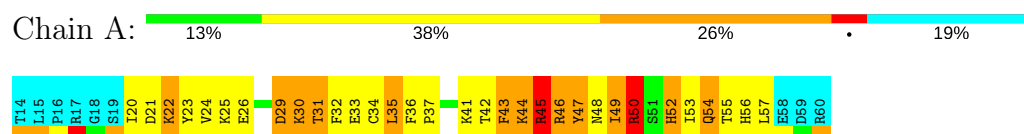
4.2.29 Score per residue for model 29

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



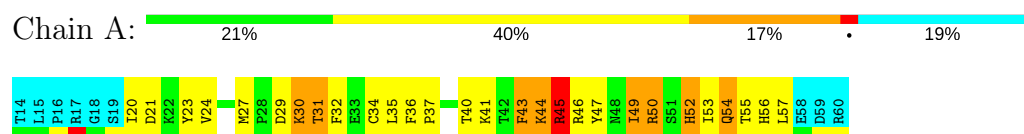
4.2.30 Score per residue for model 30

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



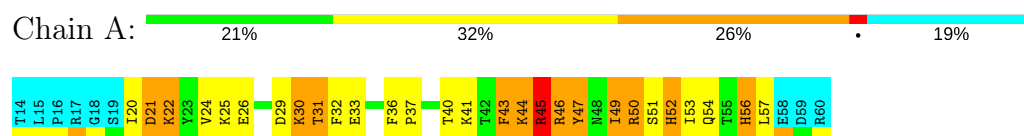
4.2.31 Score per residue for model 31

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



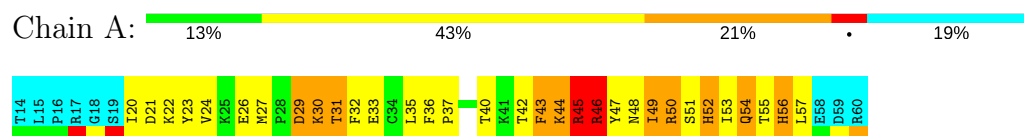
4.2.32 Score per residue for model 32

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



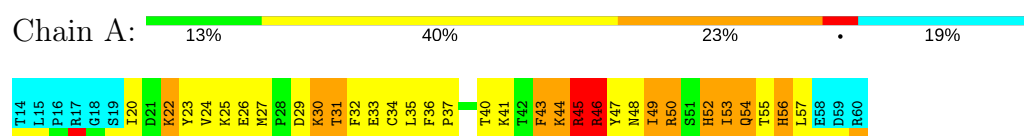
4.2.33 Score per residue for model 33

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



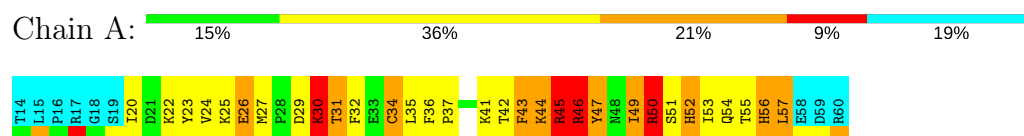
4.2.34 Score per residue for model 34

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



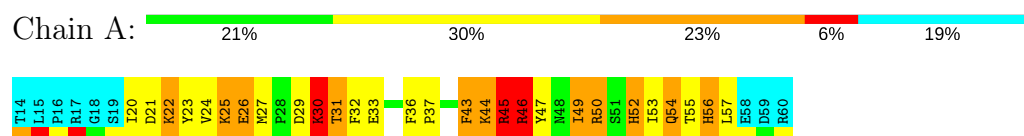
4.2.35 Score per residue for model 35

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



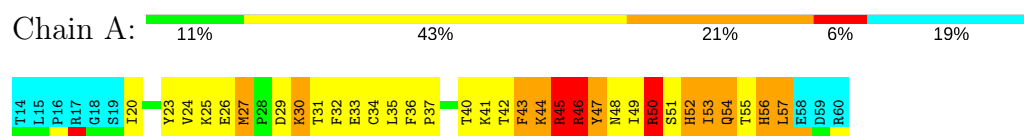
4.2.36 Score per residue for model 36

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



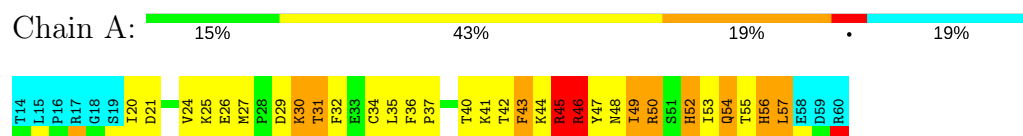
4.2.37 Score per residue for model 37

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



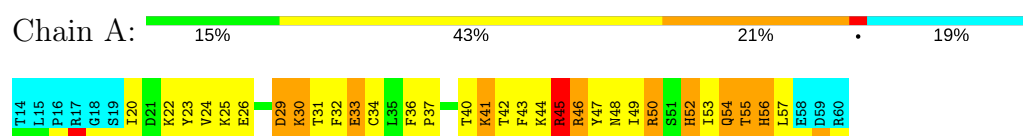
4.2.38 Score per residue for model 38

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



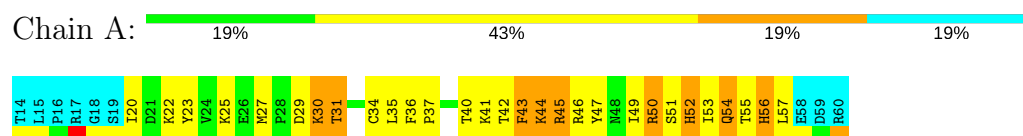
4.2.39 Score per residue for model 39

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



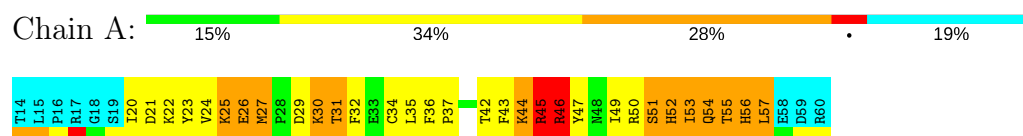
4.2.40 Score per residue for model 40

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



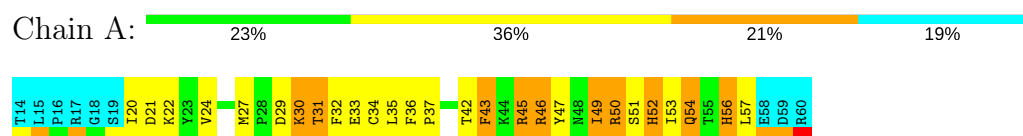
4.2.41 Score per residue for model 41

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



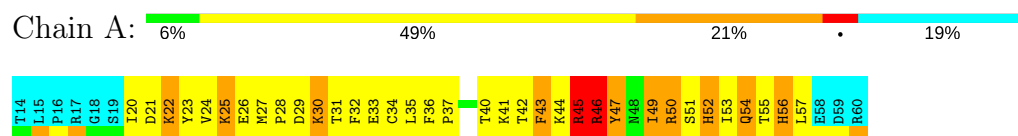
4.2.42 Score per residue for model 42

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



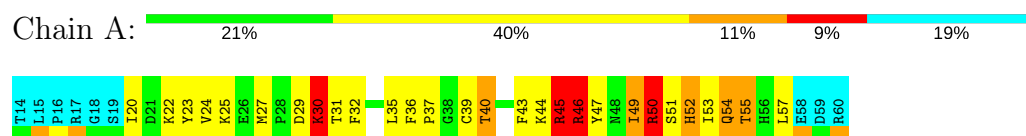
4.2.43 Score per residue for model 43

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



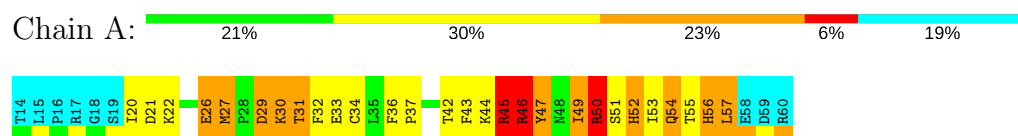
4.2.44 Score per residue for model 44

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



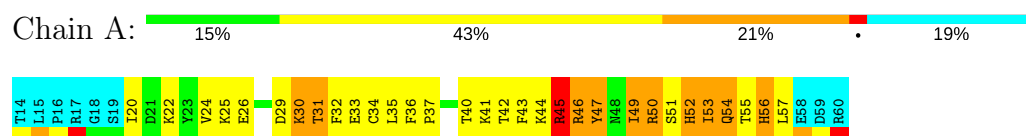
4.2.45 Score per residue for model 45

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



4.2.46 Score per residue for model 46

- Molecule 1: TRANSCRIPTIONAL FACTOR SWI5



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 46 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	3.1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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

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	2.8±0.4
All	All	0	130

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	46	ARG	Sidechain	46
1	A	45	ARG	Sidechain	43
1	A	50	ARG	Sidechain	41

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	325	328	328	48±8
All	All	14996	15088	15088	2221

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 74.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ILE:HG22	1:A:53:ILE:HD12	1.06	1.20	45	3
1:A:36:PHE:CD2	1:A:57:LEU:HD21	1.02	1.90	13	13
1:A:36:PHE:CD2	1:A:57:LEU:HD11	1.01	1.91	44	19
1:A:49:ILE:HD13	1:A:50:ARG:N	0.98	1.74	26	37
1:A:53:ILE:CG2	1:A:57:LEU:HD22	0.97	1.89	22	16
1:A:43:PHE:CE1	1:A:49:ILE:HG23	0.97	1.95	38	3
1:A:56:HIS:O	1:A:57:LEU:HD22	0.92	1.63	13	6
1:A:20:ILE:HG23	1:A:57:LEU:HD22	0.91	1.41	15	1
1:A:53:ILE:CG2	1:A:57:LEU:HD13	0.91	1.96	24	13
1:A:36:PHE:CG	1:A:57:LEU:HD11	0.91	2.00	38	11
1:A:53:ILE:HG23	1:A:57:LEU:HD13	0.89	1.43	27	11
1:A:20:ILE:HG21	1:A:54:GLN:NE2	0.88	1.83	32	6
1:A:53:ILE:HG22	1:A:57:LEU:HD13	0.86	1.43	43	8
1:A:53:ILE:HB	1:A:57:LEU:HD13	0.86	1.46	41	1
1:A:53:ILE:CG2	1:A:57:LEU:HD12	0.86	2.01	20	1
1:A:20:ILE:CG2	1:A:53:ILE:HD12	0.84	2.01	15	9
1:A:53:ILE:HG23	1:A:57:LEU:HD12	0.84	1.46	20	1
1:A:36:PHE:CD2	1:A:57:LEU:HD13	0.82	2.08	40	12
1:A:20:ILE:HD13	1:A:54:GLN:NE2	0.82	1.90	10	4
1:A:20:ILE:O	1:A:24:VAL:HG23	0.81	1.76	42	22
1:A:20:ILE:HG23	1:A:53:ILE:HD12	0.80	1.53	24	10
1:A:20:ILE:HG21	1:A:50:ARG:HG2	0.79	1.54	33	2
1:A:56:HIS:O	1:A:57:LEU:HD12	0.79	1.77	43	6
1:A:53:ILE:CB	1:A:57:LEU:HD13	0.79	2.07	41	3
1:A:53:ILE:HG22	1:A:57:LEU:HD22	0.78	1.55	27	13
1:A:49:ILE:HD12	1:A:49:ILE:N	0.77	1.95	39	3
1:A:53:ILE:HG23	1:A:57:LEU:HD23	0.77	1.56	29	6
1:A:36:PHE:CE2	1:A:57:LEU:HD13	0.77	2.15	10	10
1:A:49:ILE:N	1:A:49:ILE:HD12	0.76	1.95	37	2
1:A:53:ILE:HG22	1:A:57:LEU:CB	0.75	2.11	10	11
1:A:53:ILE:HG22	1:A:57:LEU:CD1	0.74	2.11	15	6
1:A:51:SER:O	1:A:55:THR:HG23	0.73	1.83	33	5
1:A:43:PHE:CZ	1:A:49:ILE:HG23	0.73	2.19	46	2
1:A:25:LYS:HB2	1:A:35:LEU:HD11	0.73	1.60	12	4
1:A:49:ILE:HD13	1:A:50:ARG:H	0.72	1.43	5	30
1:A:53:ILE:O	1:A:57:LEU:HD12	0.72	1.84	1	1
1:A:20:ILE:HG23	1:A:57:LEU:HB3	0.72	1.60	45	1
1:A:49:ILE:HG22	1:A:52:HIS:CD2	0.71	2.20	38	1
1:A:24:VAL:HG13	1:A:24:VAL:O	0.70	1.85	27	8
1:A:25:LYS:HD3	1:A:35:LEU:HD21	0.70	1.63	28	2
1:A:36:PHE:CE2	1:A:57:LEU:HD11	0.70	2.21	13	5
1:A:24:VAL:O	1:A:24:VAL:HG13	0.70	1.84	36	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ILE:HG22	1:A:57:LEU:HB3	0.70	1.62	10	2
1:A:36:PHE:CG	1:A:56:HIS:CE1	0.69	2.80	1	1
1:A:53:ILE:HG23	1:A:57:LEU:CD1	0.69	2.17	27	7
1:A:34:CYS:SG	1:A:53:ILE:HG23	0.69	2.28	5	6
1:A:34:CYS:SG	1:A:53:ILE:HD11	0.69	2.28	31	3
1:A:20:ILE:HD12	1:A:20:ILE:N	0.68	2.03	4	1
1:A:20:ILE:HG23	1:A:53:ILE:CD1	0.68	2.18	41	7
1:A:53:ILE:CG2	1:A:57:LEU:HD23	0.68	2.19	32	8
1:A:43:PHE:N	1:A:43:PHE:CD1	0.67	2.63	3	24
1:A:52:HIS:CD2	1:A:53:ILE:N	0.67	2.62	41	44
1:A:49:ILE:H	1:A:49:ILE:HD12	0.66	1.51	40	5
1:A:53:ILE:HG22	1:A:57:LEU:HB2	0.66	1.66	13	10
1:A:20:ILE:HG22	1:A:53:ILE:CD1	0.66	2.12	45	2
1:A:36:PHE:CD2	1:A:57:LEU:CD1	0.66	2.79	31	25
1:A:53:ILE:HG23	1:A:57:LEU:CD2	0.66	2.20	28	5
1:A:43:PHE:CD1	1:A:43:PHE:N	0.65	2.64	2	21
1:A:24:VAL:HG22	1:A:53:ILE:HD11	0.65	1.68	2	5
1:A:36:PHE:CD2	1:A:57:LEU:CD2	0.65	2.80	18	10
1:A:36:PHE:CE2	1:A:57:LEU:CD1	0.65	2.80	31	16
1:A:53:ILE:HG23	1:A:57:LEU:CB	0.65	2.21	38	1
1:A:25:LYS:HD3	1:A:35:LEU:HD11	0.65	1.67	26	1
1:A:36:PHE:HD2	1:A:57:LEU:HD13	0.64	1.52	5	7
1:A:26:GLU:CG	1:A:32:PHE:CE2	0.64	2.81	22	1
1:A:36:PHE:CD1	1:A:56:HIS:CE1	0.64	2.86	1	1
1:A:36:PHE:CD1	1:A:57:LEU:HD11	0.64	2.28	37	1
1:A:43:PHE:CG	1:A:49:ILE:CG2	0.64	2.81	1	20
1:A:21:ASP:HA	1:A:24:VAL:HG12	0.63	1.71	33	5
1:A:36:PHE:CD1	1:A:57:LEU:CD1	0.63	2.81	21	2
1:A:52:HIS:HD2	1:A:53:ILE:HG23	0.63	1.53	39	3
1:A:20:ILE:HG23	1:A:53:ILE:HB	0.63	1.70	12	2
1:A:26:GLU:CB	1:A:32:PHE:CE1	0.63	2.81	36	1
1:A:24:VAL:N	1:A:35:LEU:HD12	0.63	2.08	43	7
1:A:43:PHE:CD2	1:A:48:ASN:CB	0.62	2.82	38	1
1:A:24:VAL:HG22	1:A:53:ILE:CD1	0.62	2.24	30	4
1:A:52:HIS:O	1:A:55:THR:HG22	0.62	1.94	26	12
1:A:53:ILE:O	1:A:57:LEU:N	0.62	2.32	12	44
1:A:47:TYR:CD1	1:A:47:TYR:N	0.62	2.67	28	11
1:A:53:ILE:HG21	1:A:57:LEU:HD22	0.62	1.72	31	4
1:A:52:HIS:CD2	1:A:53:ILE:HG23	0.62	2.28	3	7
1:A:20:ILE:HD12	1:A:54:GLN:NE2	0.62	2.10	46	3
1:A:53:ILE:O	1:A:57:LEU:CB	0.62	2.48	3	21

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:LYS:HD2	1:A:35:LEU:HD21	0.61	1.72	46	2
1:A:29:ASP:O	1:A:30:LYS:CB	0.61	2.48	36	37
1:A:53:ILE:HG23	1:A:57:LEU:HB2	0.61	1.71	38	2
1:A:36:PHE:CE1	1:A:37:PRO:O	0.60	2.55	12	44
1:A:31:THR:O	1:A:32:PHE:CD2	0.60	2.54	23	26
1:A:20:ILE:N	1:A:20:ILE:HD13	0.60	2.12	2	18
1:A:25:LYS:CD	1:A:35:LEU:HD21	0.60	2.25	28	3
1:A:49:ILE:C	1:A:49:ILE:HD13	0.60	2.16	30	4
1:A:32:PHE:CE2	1:A:46:ARG:O	0.60	2.55	23	3
1:A:36:PHE:HD2	1:A:57:LEU:HD21	0.60	1.57	24	6
1:A:32:PHE:CZ	1:A:46:ARG:O	0.59	2.55	33	5
1:A:53:ILE:CG2	1:A:57:LEU:CD2	0.59	2.80	19	20
1:A:53:ILE:O	1:A:57:LEU:HB2	0.59	1.97	38	35
1:A:53:ILE:CG2	1:A:57:LEU:CB	0.59	2.79	38	2
1:A:53:ILE:HG22	1:A:57:LEU:CG	0.59	2.27	13	7
1:A:49:ILE:HD13	1:A:50:ARG:HG2	0.59	1.74	2	1
1:A:53:ILE:CG2	1:A:57:LEU:CD1	0.59	2.79	20	9
1:A:20:ILE:CD1	1:A:54:GLN:NE2	0.59	2.66	45	5
1:A:24:VAL:CG2	1:A:53:ILE:CD1	0.59	2.81	2	4
1:A:49:ILE:HD12	1:A:49:ILE:H	0.59	1.56	45	2
1:A:20:ILE:N	1:A:20:ILE:HD12	0.59	2.12	16	2
1:A:50:ARG:O	1:A:54:GLN:NE2	0.59	2.36	45	15
1:A:20:ILE:N	1:A:20:ILE:CD1	0.59	2.66	16	4
1:A:36:PHE:HD1	1:A:57:LEU:HD11	0.59	1.57	37	1
1:A:23:TYR:O	1:A:35:LEU:HD12	0.59	1.98	11	2
1:A:26:GLU:CB	1:A:32:PHE:CE2	0.58	2.86	45	2
1:A:31:THR:O	1:A:32:PHE:CD1	0.58	2.56	45	15
1:A:43:PHE:CE1	1:A:49:ILE:CG2	0.58	2.83	38	1
1:A:36:PHE:CD2	1:A:57:LEU:CG	0.58	2.87	9	13
1:A:52:HIS:C	1:A:52:HIS:CD2	0.58	2.77	4	18
1:A:40:THR:HG22	1:A:40:THR:O	0.58	1.98	18	1
1:A:49:ILE:CD1	1:A:49:ILE:N	0.58	2.67	39	1
1:A:24:VAL:HG21	1:A:50:ARG:HG2	0.57	1.74	12	1
1:A:43:PHE:CD2	1:A:48:ASN:HB2	0.57	2.35	38	1
1:A:39:CYS:O	1:A:40:THR:CB	0.57	2.50	44	1
1:A:52:HIS:CD2	1:A:52:HIS:C	0.57	2.77	14	17
1:A:49:ILE:HG22	1:A:53:ILE:HG12	0.57	1.77	40	2
1:A:49:ILE:HD13	1:A:49:ILE:C	0.57	2.19	20	10
1:A:22:LYS:CD	1:A:23:TYR:CD2	0.57	2.88	19	1
1:A:24:VAL:CG2	1:A:53:ILE:HD11	0.56	2.30	2	3
1:A:20:ILE:HD13	1:A:20:ILE:N	0.56	2.13	18	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:HIS:CE1	1:A:56:HIS:CD2	0.56	2.93	38	5
1:A:20:ILE:HD13	1:A:57:LEU:HD22	0.56	1.75	41	1
1:A:20:ILE:HD13	1:A:54:GLN:OE1	0.56	2.01	24	1
1:A:36:PHE:CE2	1:A:57:LEU:HG	0.56	2.35	44	11
1:A:36:PHE:CE2	1:A:57:LEU:CG	0.56	2.89	44	2
1:A:49:ILE:N	1:A:49:ILE:CD1	0.56	2.69	37	2
1:A:22:LYS:O	1:A:23:TYR:CD1	0.56	2.58	36	10
1:A:53:ILE:CG2	1:A:57:LEU:HB2	0.56	2.30	38	5
1:A:57:LEU:H	1:A:57:LEU:HD12	0.56	1.61	1	1
1:A:36:PHE:CB	1:A:57:LEU:HD11	0.55	2.31	38	1
1:A:26:GLU:HB3	1:A:32:PHE:CE2	0.55	2.36	45	1
1:A:43:PHE:CD1	1:A:49:ILE:HG12	0.55	2.36	43	3
1:A:20:ILE:CG2	1:A:54:GLN:NE2	0.55	2.69	5	3
1:A:41:LYS:O	1:A:43:PHE:CZ	0.55	2.60	5	1
1:A:47:TYR:N	1:A:47:TYR:CD1	0.55	2.75	6	6
1:A:20:ILE:CD1	1:A:20:ILE:N	0.55	2.69	26	4
1:A:26:GLU:HG3	1:A:32:PHE:CE2	0.55	2.37	22	1
1:A:34:CYS:SG	1:A:53:ILE:CG1	0.55	2.95	31	1
1:A:44:LYS:O	1:A:45:ARG:CB	0.55	2.54	12	2
1:A:49:ILE:CD1	1:A:50:ARG:N	0.55	2.67	9	23
1:A:23:TYR:CZ	1:A:37:PRO:HD3	0.55	2.36	44	9
1:A:42:THR:C	1:A:43:PHE:CD1	0.55	2.80	38	12
1:A:34:CYS:SG	1:A:53:ILE:CG2	0.55	2.95	3	14
1:A:24:VAL:HG23	1:A:49:ILE:HD11	0.55	1.78	36	1
1:A:36:PHE:CG	1:A:37:PRO:HD2	0.54	2.37	35	43
1:A:49:ILE:O	1:A:52:HIS:N	0.54	2.40	46	8
1:A:52:HIS:O	1:A:55:THR:CG2	0.54	2.55	11	6
1:A:27:MET:CB	1:A:31:THR:HG23	0.54	2.32	34	1
1:A:36:PHE:CD2	1:A:57:LEU:HG	0.54	2.38	43	10
1:A:36:PHE:HD2	1:A:57:LEU:HD22	0.54	1.61	42	1
1:A:53:ILE:HG23	1:A:57:LEU:HD22	0.54	1.71	22	2
1:A:31:THR:O	1:A:32:PHE:CG	0.54	2.61	12	1
1:A:34:CYS:HB2	1:A:49:ILE:HG21	0.54	1.80	38	1
1:A:26:GLU:CB	1:A:32:PHE:CZ	0.54	2.90	20	8
1:A:20:ILE:HD13	1:A:54:GLN:CD	0.54	2.23	10	3
1:A:42:THR:O	1:A:43:PHE:CG	0.54	2.61	39	1
1:A:24:VAL:CG1	1:A:24:VAL:O	0.53	2.55	27	6
1:A:50:ARG:O	1:A:53:ILE:CG1	0.53	2.56	3	1
1:A:26:GLU:HG2	1:A:32:PHE:CE1	0.53	2.39	38	1
1:A:30:LYS:C	1:A:31:THR:HG22	0.53	2.23	34	2
1:A:20:ILE:O	1:A:24:VAL:CG2	0.53	2.57	20	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:ASP:CG	1:A:31:THR:HG1	0.53	2.06	11	6
1:A:41:LYS:O	1:A:43:PHE:CE1	0.53	2.62	2	3
1:A:29:ASP:O	1:A:30:LYS:CG	0.53	2.56	36	3
1:A:53:ILE:HG22	1:A:57:LEU:CD2	0.53	2.32	36	13
1:A:56:HIS:O	1:A:56:HIS:ND1	0.53	2.41	43	25
1:A:22:LYS:CG	1:A:22:LYS:O	0.53	2.57	23	2
1:A:23:TYR:O	1:A:35:LEU:CD1	0.53	2.57	11	2
1:A:26:GLU:HB2	1:A:32:PHE:CZ	0.53	2.38	45	3
1:A:24:VAL:O	1:A:24:VAL:CG1	0.53	2.56	33	10
1:A:27:MET:CG	1:A:29:ASP:OD1	0.53	2.57	40	4
1:A:43:PHE:CE1	1:A:49:ILE:HG13	0.53	2.39	40	1
1:A:57:LEU:CG	1:A:57:LEU:O	0.53	2.56	42	1
1:A:56:HIS:CG	1:A:56:HIS:O	0.53	2.62	5	8
1:A:56:HIS:ND1	1:A:56:HIS:O	0.53	2.41	14	16
1:A:26:GLU:HB3	1:A:32:PHE:CZ	0.53	2.38	27	4
1:A:43:PHE:CD1	1:A:49:ILE:HB	0.53	2.39	33	13
1:A:53:ILE:O	1:A:57:LEU:HB3	0.52	2.04	42	8
1:A:32:PHE:CD1	1:A:49:ILE:HD12	0.52	2.39	33	2
1:A:53:ILE:O	1:A:55:THR:N	0.52	2.43	13	19
1:A:20:ILE:CG2	1:A:53:ILE:CD1	0.52	2.87	41	4
1:A:36:PHE:CD1	1:A:36:PHE:C	0.52	2.82	23	8
1:A:49:ILE:O	1:A:50:ARG:C	0.52	2.47	46	8
1:A:43:PHE:CD2	1:A:49:ILE:HG13	0.52	2.40	39	1
1:A:24:VAL:CG2	1:A:53:ILE:HD12	0.52	2.33	20	2
1:A:49:ILE:HD13	1:A:50:ARG:HG3	0.52	1.82	24	1
1:A:20:ILE:HG12	1:A:54:GLN:NE2	0.52	2.19	26	3
1:A:36:PHE:CD1	1:A:37:PRO:HD2	0.52	2.40	42	6
1:A:26:GLU:O	1:A:26:GLU:CG	0.52	2.58	30	5
1:A:29:ASP:O	1:A:30:LYS:HB2	0.52	2.04	34	46
1:A:44:LYS:O	1:A:45:ARG:CG	0.52	2.58	6	3
1:A:44:LYS:O	1:A:46:ARG:N	0.52	2.42	34	8
1:A:26:GLU:CG	1:A:32:PHE:CZ	0.52	2.93	22	3
1:A:34:CYS:SG	1:A:53:ILE:CD1	0.52	2.98	31	6
1:A:27:MET:CB	1:A:29:ASP:OD1	0.52	2.57	37	7
1:A:49:ILE:O	1:A:51:SER:N	0.52	2.42	46	7
1:A:26:GLU:HA	1:A:32:PHE:CE2	0.51	2.40	34	1
1:A:56:HIS:O	1:A:56:HIS:CG	0.51	2.62	37	18
1:A:45:ARG:O	1:A:46:ARG:CB	0.51	2.57	35	6
1:A:26:GLU:HB3	1:A:32:PHE:CE1	0.51	2.41	27	5
1:A:26:GLU:HA	1:A:32:PHE:CE1	0.51	2.40	23	4
1:A:42:THR:C	1:A:43:PHE:CG	0.51	2.84	45	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:ASP:OD1	1:A:31:THR:CG2	0.51	2.58	34	2
1:A:46:ARG:C	1:A:47:TYR:CD1	0.51	2.84	29	1
1:A:43:PHE:CE1	1:A:49:ILE:HB	0.51	2.41	34	31
1:A:41:LYS:O	1:A:43:PHE:CE2	0.51	2.64	39	1
1:A:25:LYS:HD2	1:A:35:LEU:HD11	0.50	1.83	41	1
1:A:43:PHE:CG	1:A:49:ILE:HB	0.50	2.41	30	7
1:A:31:THR:HG22	1:A:32:PHE:H	0.50	1.66	8	21
1:A:53:ILE:O	1:A:56:HIS:HB2	0.50	2.06	1	1
1:A:23:TYR:CD1	1:A:35:LEU:O	0.50	2.65	23	1
1:A:32:PHE:N	1:A:43:PHE:O	0.50	2.44	34	13
1:A:52:HIS:CD2	1:A:53:ILE:HG13	0.50	2.41	31	1
1:A:53:ILE:O	1:A:57:LEU:CA	0.50	2.60	42	1
1:A:36:PHE:CE1	1:A:57:LEU:HG	0.50	2.41	37	1
1:A:21:ASP:OD1	1:A:21:ASP:N	0.50	2.44	32	2
1:A:39:CYS:O	1:A:40:THR:OG1	0.50	2.30	44	1
1:A:50:ARG:CG	1:A:51:SER:N	0.49	2.74	1	2
1:A:49:ILE:O	1:A:53:ILE:CG1	0.49	2.61	42	3
1:A:25:LYS:HG3	1:A:35:LEU:HD21	0.49	1.83	7	2
1:A:57:LEU:HG	1:A:57:LEU:O	0.49	2.07	42	1
1:A:26:GLU:HA	1:A:32:PHE:CD1	0.49	2.43	12	4
1:A:36:PHE:C	1:A:36:PHE:CD1	0.49	2.86	10	11
1:A:25:LYS:CG	1:A:35:LEU:HD11	0.49	2.38	7	2
1:A:23:TYR:C	1:A:35:LEU:HD12	0.49	2.27	43	2
1:A:43:PHE:CZ	1:A:49:ILE:HB	0.49	2.43	25	9
1:A:53:ILE:CG2	1:A:57:LEU:HG	0.49	2.38	28	7
1:A:53:ILE:O	1:A:57:LEU:CD1	0.49	2.59	1	1
1:A:30:LYS:C	1:A:31:THR:CG2	0.49	2.80	36	2
1:A:49:ILE:HG22	1:A:52:HIS:HD2	0.49	1.62	38	3
1:A:36:PHE:CE2	1:A:57:LEU:HD21	0.49	2.42	20	3
1:A:36:PHE:CD2	1:A:37:PRO:HD2	0.49	2.43	13	15
1:A:25:LYS:CB	1:A:33:GLU:O	0.49	2.60	37	2
1:A:23:TYR:CD1	1:A:35:LEU:HD12	0.49	2.43	30	1
1:A:53:ILE:O	1:A:54:GLN:C	0.49	2.51	15	28
1:A:26:GLU:CG	1:A:26:GLU:O	0.48	2.61	43	3
1:A:49:ILE:C	1:A:49:ILE:CD1	0.48	2.81	30	4
1:A:45:ARG:CG	1:A:46:ARG:N	0.48	2.75	12	1
1:A:45:ARG:O	1:A:46:ARG:CG	0.48	2.61	41	1
1:A:23:TYR:CE1	1:A:37:PRO:HD3	0.48	2.43	35	16
1:A:23:TYR:CD1	1:A:36:PHE:HA	0.48	2.43	31	8
1:A:25:LYS:N	1:A:35:LEU:HD11	0.48	2.24	20	2
1:A:24:VAL:C	1:A:35:LEU:HD12	0.48	2.28	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:ILE:O	1:A:53:ILE:HG12	0.48	2.09	37	7
1:A:20:ILE:HD13	1:A:57:LEU:HD23	0.48	1.86	39	3
1:A:24:VAL:CG2	1:A:49:ILE:HD11	0.48	2.39	36	2
1:A:49:ILE:CD1	1:A:49:ILE:C	0.48	2.82	20	6
1:A:43:PHE:CD1	1:A:49:ILE:HG13	0.48	2.43	20	5
1:A:25:LYS:O	1:A:32:PHE:CD2	0.48	2.67	46	1
1:A:20:ILE:CG2	1:A:50:ARG:CG	0.48	2.92	23	2
1:A:23:TYR:O	1:A:35:LEU:CG	0.48	2.62	11	2
1:A:24:VAL:N	1:A:35:LEU:CD1	0.48	2.77	43	1
1:A:43:PHE:CD1	1:A:49:ILE:CG1	0.48	2.96	43	3
1:A:22:LYS:O	1:A:23:TYR:CG	0.47	2.67	14	6
1:A:55:THR:CG2	1:A:56:HIS:N	0.47	2.76	6	1
1:A:44:LYS:O	1:A:45:ARG:HB2	0.47	2.08	12	4
1:A:26:GLU:HG3	1:A:32:PHE:CZ	0.47	2.43	14	1
1:A:53:ILE:HG23	1:A:57:LEU:CG	0.47	2.39	35	1
1:A:20:ILE:HG13	1:A:53:ILE:CG2	0.47	2.38	24	3
1:A:36:PHE:CD1	1:A:57:LEU:HD12	0.47	2.44	21	1
1:A:49:ILE:O	1:A:53:ILE:HB	0.47	2.09	38	1
1:A:29:ASP:OD2	1:A:31:THR:OG1	0.47	2.33	17	14
1:A:21:ASP:N	1:A:21:ASP:OD1	0.47	2.48	43	1
1:A:36:PHE:CE2	1:A:57:LEU:HD12	0.47	2.44	31	2
1:A:25:LYS:CG	1:A:35:LEU:HD21	0.47	2.40	19	1
1:A:50:ARG:HG3	1:A:51:SER:N	0.47	2.25	1	3
1:A:20:ILE:CG2	1:A:50:ARG:HG3	0.47	2.38	23	1
1:A:26:GLU:HB2	1:A:32:PHE:CE1	0.47	2.45	36	1
1:A:32:PHE:CD2	1:A:49:ILE:HD11	0.47	2.45	38	1
1:A:43:PHE:CD2	1:A:48:ASN:HB3	0.47	2.44	38	1
1:A:25:LYS:CB	1:A:35:LEU:HD11	0.47	2.40	16	3
1:A:25:LYS:N	1:A:35:LEU:HD12	0.47	2.24	2	1
1:A:26:GLU:HG2	1:A:32:PHE:CE2	0.47	2.44	18	2
1:A:29:ASP:O	1:A:30:LYS:HG3	0.47	2.09	34	2
1:A:24:VAL:C	1:A:35:LEU:CD1	0.47	2.83	3	1
1:A:43:PHE:CD1	1:A:49:ILE:HG21	0.47	2.45	1	5
1:A:22:LYS:HE2	1:A:23:TYR:CE2	0.47	2.45	7	2
1:A:22:LYS:HD2	1:A:23:TYR:CD2	0.47	2.45	19	1
1:A:25:LYS:HB3	1:A:33:GLU:CB	0.47	2.40	39	3
1:A:43:PHE:CD2	1:A:49:ILE:HB	0.46	2.45	30	2
1:A:20:ILE:CD1	1:A:54:GLN:HG3	0.46	2.40	12	4
1:A:23:TYR:CG	1:A:36:PHE:HA	0.46	2.45	43	3
1:A:43:PHE:CG	1:A:49:ILE:HG21	0.46	2.44	35	19
1:A:29:ASP:OD1	1:A:31:THR:OG1	0.46	2.33	6	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ILE:CG2	1:A:53:ILE:HB	0.46	2.39	45	2
1:A:23:TYR:CE2	1:A:37:PRO:HD3	0.46	2.45	23	1
1:A:29:ASP:OD1	1:A:31:THR:HG22	0.46	2.10	34	1
1:A:27:MET:SD	1:A:29:ASP:OD2	0.46	2.73	36	1
1:A:30:LYS:O	1:A:44:LYS:CB	0.46	2.63	12	3
1:A:40:THR:O	1:A:40:THR:HG22	0.46	2.11	34	1
1:A:30:LYS:O	1:A:44:LYS:HB2	0.46	2.10	36	7
1:A:27:MET:HB2	1:A:29:ASP:OD1	0.46	2.11	4	4
1:A:29:ASP:OD2	1:A:31:THR:HG23	0.46	2.10	36	1
1:A:20:ILE:HD11	1:A:54:GLN:HG3	0.46	1.88	29	2
1:A:41:LYS:HG2	1:A:43:PHE:CE2	0.46	2.46	29	1
1:A:43:PHE:HB2	1:A:49:ILE:CG2	0.46	2.41	33	1
1:A:44:LYS:O	1:A:45:ARG:O	0.46	2.34	32	4
1:A:47:TYR:O	1:A:50:ARG:CG	0.46	2.64	37	1
1:A:50:ARG:O	1:A:53:ILE:HG12	0.46	2.10	3	1
1:A:44:LYS:O	1:A:45:ARG:C	0.46	2.54	31	31
1:A:27:MET:HB3	1:A:29:ASP:OD1	0.46	2.11	37	16
1:A:43:PHE:CE2	1:A:49:ILE:HB	0.46	2.46	14	3
1:A:57:LEU:HD12	1:A:57:LEU:O	0.46	2.10	42	1
1:A:44:LYS:O	1:A:45:ARG:HG3	0.45	2.11	6	2
1:A:56:HIS:CE1	1:A:57:LEU:CD1	0.45	2.99	22	1
1:A:20:ILE:CG1	1:A:54:GLN:NE2	0.45	2.80	26	1
1:A:45:ARG:HG2	1:A:46:ARG:N	0.45	2.26	12	1
1:A:52:HIS:O	1:A:55:THR:OG1	0.45	2.33	27	1
1:A:24:VAL:HG22	1:A:53:ILE:HD12	0.45	1.87	20	2
1:A:36:PHE:CD1	1:A:37:PRO:O	0.45	2.70	1	5
1:A:31:THR:OG1	1:A:32:PHE:N	0.45	2.49	34	1
1:A:27:MET:HG3	1:A:29:ASP:OD1	0.45	2.11	27	1
1:A:20:ILE:HG22	1:A:50:ARG:HG3	0.45	1.88	46	1
1:A:50:ARG:O	1:A:54:GLN:CD	0.45	2.55	42	1
1:A:53:ILE:HG22	1:A:57:LEU:HD21	0.45	1.88	46	1
1:A:43:PHE:HB2	1:A:49:ILE:HD11	0.45	1.88	39	1
1:A:27:MET:SD	1:A:29:ASP:OD1	0.45	2.75	3	1
1:A:53:ILE:HG22	1:A:57:LEU:HD23	0.45	1.87	19	1
1:A:53:ILE:O	1:A:57:LEU:C	0.45	2.55	42	1
1:A:53:ILE:O	1:A:56:HIS:N	0.45	2.50	15	8
1:A:27:MET:CB	1:A:31:THR:HB	0.45	2.42	10	6
1:A:51:SER:O	1:A:55:THR:OG1	0.45	2.34	7	1
1:A:41:LYS:HG2	1:A:43:PHE:CZ	0.45	2.46	29	1
1:A:27:MET:CG	1:A:28:PRO:HD2	0.45	2.41	43	2
1:A:32:PHE:CD1	1:A:44:LYS:O	0.45	2.69	41	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ILE:HA	1:A:57:LEU:CD2	0.45	2.42	15	1
1:A:26:GLU:HG2	1:A:32:PHE:CZ	0.45	2.46	22	1
1:A:20:ILE:CD1	1:A:57:LEU:HB3	0.44	2.42	43	1
1:A:36:PHE:CD1	1:A:37:PRO:N	0.44	2.84	46	5
1:A:40:THR:O	1:A:40:THR:CG2	0.44	2.65	44	2
1:A:22:LYS:CD	1:A:23:TYR:CE2	0.44	3.00	19	1
1:A:20:ILE:HG13	1:A:54:GLN:NE2	0.44	2.27	31	6
1:A:36:PHE:CG	1:A:57:LEU:HD21	0.44	2.39	13	2
1:A:44:LYS:C	1:A:45:ARG:CG	0.44	2.86	6	1
1:A:20:ILE:CG2	1:A:57:LEU:HD22	0.44	2.27	15	1
1:A:53:ILE:CG2	1:A:57:LEU:CG	0.44	2.95	28	5
1:A:36:PHE:CD1	1:A:37:PRO:CD	0.44	3.01	42	4
1:A:27:MET:CE	1:A:31:THR:HB	0.44	2.43	45	1
1:A:25:LYS:HB3	1:A:33:GLU:O	0.44	2.13	3	1
1:A:30:LYS:O	1:A:31:THR:HG22	0.44	2.13	36	1
1:A:30:LYS:CB	1:A:30:LYS:NZ	0.44	2.80	16	1
1:A:49:ILE:O	1:A:53:ILE:HG13	0.44	2.12	38	1
1:A:31:THR:CA	1:A:44:LYS:HA	0.44	2.43	34	4
1:A:42:THR:C	1:A:43:PHE:CD2	0.43	2.92	39	1
1:A:20:ILE:CD1	1:A:57:LEU:HD23	0.43	2.43	11	1
1:A:56:HIS:C	1:A:57:LEU:HD12	0.43	2.32	43	1
1:A:57:LEU:CD1	1:A:57:LEU:O	0.43	2.67	42	1
1:A:27:MET:CG	1:A:31:THR:HB	0.43	2.43	19	5
1:A:25:LYS:CD	1:A:33:GLU:OE1	0.43	2.66	34	1
1:A:49:ILE:CD1	1:A:49:ILE:H	0.43	2.26	38	2
1:A:29:ASP:CG	1:A:31:THR:OG1	0.43	2.57	11	3
1:A:44:LYS:O	1:A:45:ARG:HG2	0.43	2.12	31	1
1:A:27:MET:HB2	1:A:31:THR:HG23	0.43	1.88	34	1
1:A:50:ARG:O	1:A:53:ILE:HG13	0.43	2.14	8	2
1:A:51:SER:O	1:A:52:HIS:C	0.43	2.57	35	3
1:A:26:GLU:HG2	1:A:26:GLU:O	0.43	2.14	11	2
1:A:20:ILE:HG21	1:A:50:ARG:CG	0.43	2.44	23	1
1:A:25:LYS:HB2	1:A:35:LEU:CD1	0.43	2.43	16	1
1:A:49:ILE:C	1:A:51:SER:N	0.43	2.70	46	3
1:A:43:PHE:CD1	1:A:49:ILE:CG2	0.43	3.01	23	2
1:A:21:ASP:HA	1:A:24:VAL:CG1	0.43	2.44	27	1
1:A:23:TYR:O	1:A:35:LEU:HG	0.43	2.14	11	2
1:A:22:LYS:HG2	1:A:22:LYS:O	0.43	2.14	44	1
1:A:22:LYS:HD3	1:A:23:TYR:CE2	0.43	2.49	19	1
1:A:20:ILE:HG21	1:A:54:GLN:HE22	0.43	1.74	36	2
1:A:45:ARG:O	1:A:46:ARG:HB3	0.43	2.14	35	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:GLU:O	1:A:26:GLU:HG2	0.43	2.14	39	1
1:A:20:ILE:HD13	1:A:57:LEU:CD2	0.43	2.44	39	1
1:A:30:LYS:HB2	1:A:30:LYS:NZ	0.42	2.29	16	1
1:A:47:TYR:CB	1:A:50:ARG:HD3	0.42	2.44	1	1
1:A:30:LYS:O	1:A:44:LYS:HG3	0.42	2.14	45	1
1:A:45:ARG:O	1:A:46:ARG:HG3	0.42	2.14	3	1
1:A:49:ILE:CD1	1:A:50:ARG:HG3	0.42	2.44	24	1
1:A:26:GLU:O	1:A:26:GLU:CD	0.42	2.57	34	1
1:A:53:ILE:C	1:A:55:THR:N	0.42	2.72	15	9
1:A:44:LYS:O	1:A:44:LYS:HG2	0.42	2.14	44	1
1:A:20:ILE:CD1	1:A:57:LEU:HD22	0.42	2.44	41	1
1:A:25:LYS:HB2	1:A:33:GLU:O	0.42	2.14	39	2
1:A:45:ARG:HG3	1:A:46:ARG:N	0.42	2.30	33	1
1:A:57:LEU:N	1:A:57:LEU:HD12	0.42	2.28	1	1
1:A:44:LYS:C	1:A:45:ARG:HG2	0.42	2.35	6	1
1:A:30:LYS:O	1:A:44:LYS:HG2	0.42	2.14	18	1
1:A:32:PHE:CD2	1:A:49:ILE:CD1	0.42	3.02	41	1
1:A:53:ILE:HG22	1:A:57:LEU:HG	0.42	1.91	13	2
1:A:29:ASP:C	1:A:29:ASP:OD1	0.42	2.57	42	1
1:A:43:PHE:CD1	1:A:49:ILE:CB	0.42	3.03	24	3
1:A:25:LYS:HG3	1:A:27:MET:HE1	0.42	1.90	6	1
1:A:23:TYR:HB3	1:A:36:PHE:N	0.42	2.30	36	2
1:A:23:TYR:HA	1:A:35:LEU:CD1	0.42	2.44	13	1
1:A:53:ILE:HG21	1:A:57:LEU:HD23	0.42	1.91	10	1
1:A:25:LYS:O	1:A:32:PHE:CD1	0.41	2.72	36	1
1:A:25:LYS:CB	1:A:33:GLU:HB3	0.41	2.45	32	1
1:A:48:ASN:O	1:A:49:ILE:C	0.41	2.57	30	1
1:A:43:PHE:CG	1:A:49:ILE:HG22	0.41	2.49	1	1
1:A:20:ILE:HG13	1:A:54:GLN:OE1	0.41	2.15	28	1
1:A:22:LYS:HG3	1:A:23:TYR:CD2	0.41	2.50	30	1
1:A:56:HIS:CE1	1:A:57:LEU:HD12	0.41	2.50	38	1
1:A:35:LEU:O	1:A:36:PHE:C	0.41	2.58	30	1
1:A:31:THR:HA	1:A:44:LYS:CB	0.41	2.46	9	2
1:A:53:ILE:HG23	1:A:57:LEU:HG	0.41	1.92	35	1
1:A:34:CYS:SG	1:A:53:ILE:HG12	0.41	2.56	35	6
1:A:32:PHE:CD2	1:A:49:ILE:HD13	0.41	2.50	41	1
1:A:55:THR:OG1	1:A:56:HIS:N	0.41	2.53	37	1
1:A:25:LYS:HG3	1:A:35:LEU:HD22	0.41	1.91	30	1
1:A:52:HIS:CG	1:A:53:ILE:N	0.41	2.89	43	2
1:A:42:THR:O	1:A:43:PHE:CD1	0.41	2.73	39	1
1:A:22:LYS:HD3	1:A:23:TYR:CD2	0.41	2.51	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:LYS:O	1:A:22:LYS:HG3	0.41	2.15	33	1
1:A:25:LYS:HG3	1:A:35:LEU:HD11	0.41	1.91	5	2
1:A:43:PHE:C	1:A:44:LYS:CG	0.41	2.89	16	1
1:A:31:THR:HA	1:A:44:LYS:HA	0.41	1.93	34	2
1:A:20:ILE:HD13	1:A:54:GLN:CG	0.41	2.46	12	1
1:A:44:LYS:HG2	1:A:44:LYS:O	0.41	2.16	5	1
1:A:25:LYS:N	1:A:35:LEU:CD1	0.41	2.84	19	1
1:A:27:MET:HB2	1:A:31:THR:OG1	0.41	2.16	36	1
1:A:45:ARG:O	1:A:46:ARG:HB2	0.40	2.16	37	2
1:A:29:ASP:OD1	1:A:29:ASP:C	0.40	2.57	32	1
1:A:33:GLU:O	1:A:35:LEU:N	0.40	2.54	30	1
1:A:26:GLU:CG	1:A:32:PHE:CE1	0.40	3.03	38	1
1:A:45:ARG:HG3	1:A:45:ARG:O	0.40	2.17	31	1
1:A:20:ILE:HG13	1:A:53:ILE:HB	0.40	1.94	4	1
1:A:25:LYS:HG3	1:A:27:MET:CE	0.40	2.46	6	1
1:A:20:ILE:HD12	1:A:54:GLN:CD	0.40	2.36	15	1
1:A:27:MET:HG2	1:A:29:ASP:OD1	0.40	2.17	43	1
1:A:45:ARG:HG2	1:A:45:ARG:O	0.40	2.16	40	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	38/47 (81%)	29±2 (76±4%)	7±2 (19±4%)	2±1 (4±2%)	6	31
All	All	1748/2162 (81%)	1337 (76%)	338 (19%)	73 (4%)	6	31

All 7 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	45	ARG	27
1	A	30	LYS	27
1	A	46	ARG	8
1	A	54	GLN	5

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Mol	Chain	Res	Type	Models (Total)
1	A	34	CYS	3
1	A	40	THR	2
1	A	24	VAL	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	37/45 (82%)	23±2 (62±4%)	14±2 (38±4%)	1	6
All	All	1702/2070 (82%)	1047 (62%)	655 (38%)	1	6

All 30 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	47	TYR	46
1	A	52	HIS	46
1	A	54	GLN	42
1	A	56	HIS	42
1	A	49	ILE	42
1	A	43	PHE	41
1	A	46	ARG	32
1	A	45	ARG	29
1	A	25	LYS	27
1	A	22	LYS	26
1	A	40	THR	25
1	A	31	THR	25
1	A	44	LYS	23
1	A	55	THR	23
1	A	27	MET	22
1	A	41	LYS	22
1	A	33	GLU	20
1	A	26	GLU	17
1	A	57	LEU	15
1	A	50	ARG	14
1	A	30	LYS	14
1	A	35	LEU	13

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Mol	Chain	Res	Type	Models (Total)
1	A	21	ASP	13
1	A	53	ILE	11
1	A	29	ASP	9
1	A	48	ASN	7
1	A	51	SER	6
1	A	23	TYR	1
1	A	32	PHE	1
1	A	20	ILE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided