



Full wwPDB NMR Structure Validation Report ⓘ

Feb 17, 2022 – 09:53 AM EST

PDB ID : 1PE3
Title : Solution structure of the disulphide-linked dimer of human intestinal trefoil factor (TFF3)
Authors : Muskett, F.W.; May, F.E.; Westley, B.R.; Feeney, J.
Deposited on : 2003-05-21

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

MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.26
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

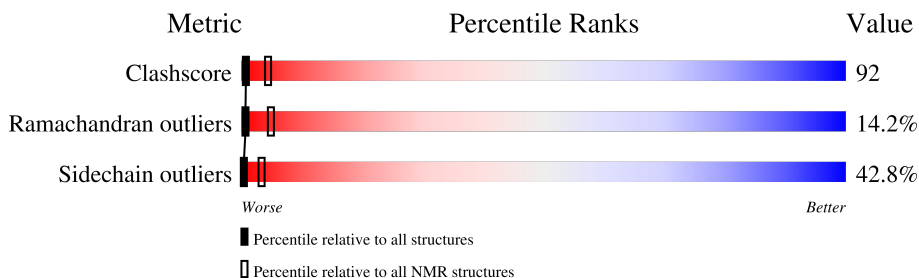
1 Overall quality at a glance

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	1	59	
1	2	59	

2 Ensemble composition and analysis

This entry contains 47 models. Model 39 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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	1:7-1:59, 2:7-2:59 (106)	0.40	39

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

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

NmrClust was unable to cluster the ensemble.

Error message: NMCparsrange - Unexpected character.

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1756 atoms, of which 842 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Trefoil factor 3.

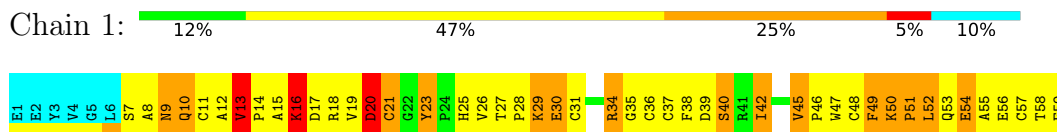
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	1	59	878	285	421	79	86	7	0
1	2	59	878	285	421	79	86	7	0

4 Residue-property plots [i](#)

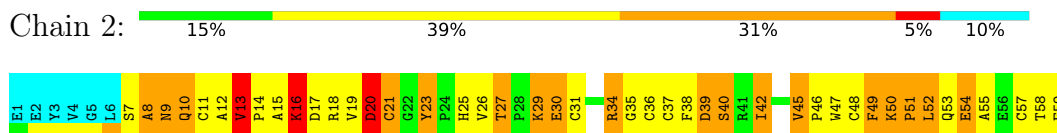
4.1 Average score per residue in the NMR ensemble

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: Trefoil factor 3



- Molecule 1: Trefoil factor 3

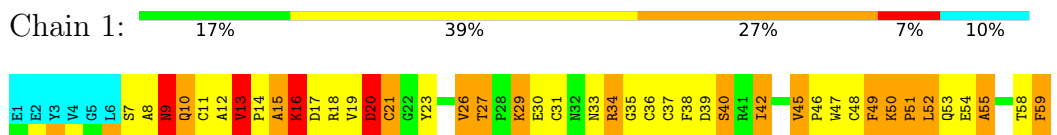


4.2 Scores per residue for each member of the ensemble

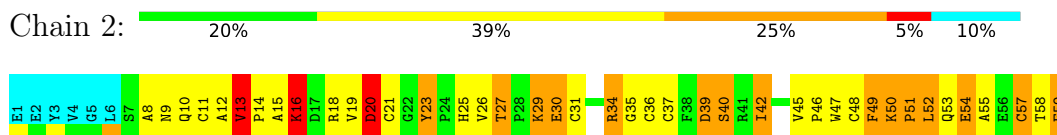
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Trefoil factor 3

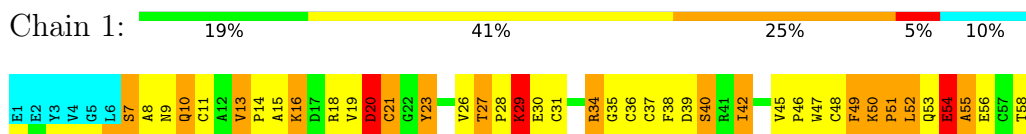


- Molecule 1: Trefoil factor 3

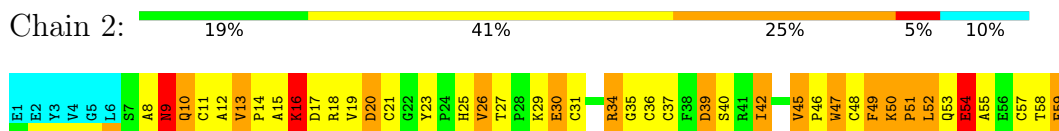


4.2.2 Score per residue for model 2

- Molecule 1: Trefoil factor 3

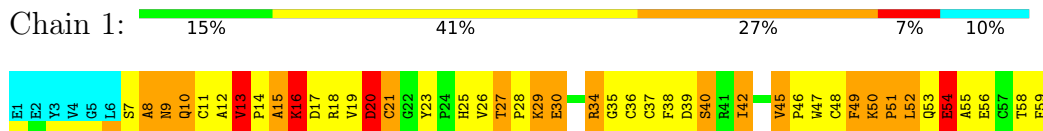


- Molecule 1: Trefoil factor 3

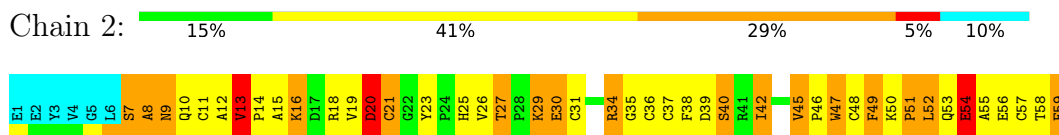


4.2.3 Score per residue for model 3

- Molecule 1: Trefoil factor 3

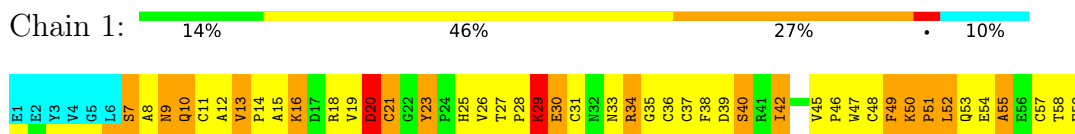


- Molecule 1: Trefoil factor 3

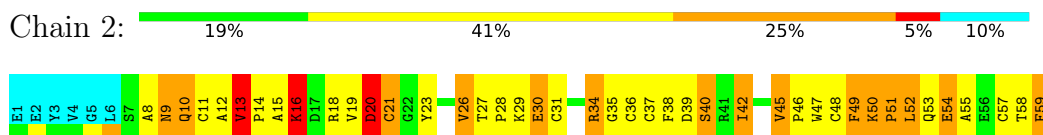


4.2.4 Score per residue for model 4

- Molecule 1: Trefoil factor 3




- Molecule 1: Trefoil factor 3



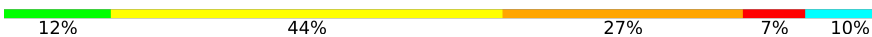
4.2.5 Score per residue for model 5

- Molecule 1: Trefoil factor 3

Chain 1: 



- Molecule 1: Trefoil factor 3

Chain 2: 



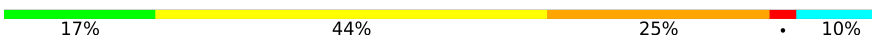
4.2.6 Score per residue for model 6

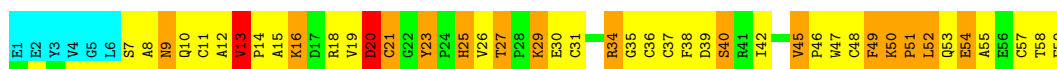
- Molecule 1: Trefoil factor 3

Chain 1: 




- Molecule 1: Trefoil factor 3

Chain 2: 



4.2.7 Score per residue for model 7

- Molecule 1: Trefoil factor 3

Chain 1: 



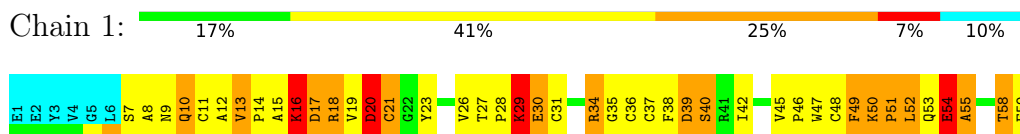
- Molecule 1: Trefoil factor 3

Chain 2: 

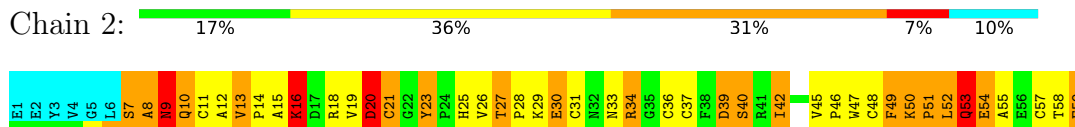


4.2.8 Score per residue for model 8

- Molecule 1: Trefoil factor 3

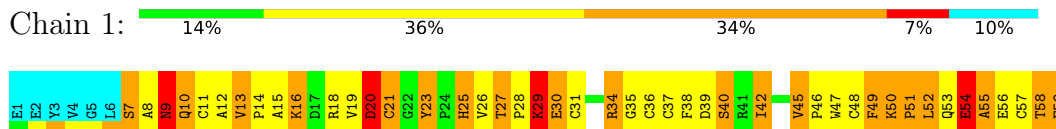


- Molecule 1: Trefoil factor 3

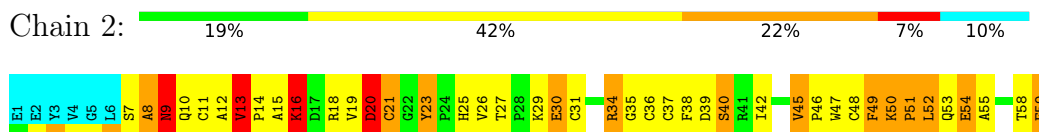


4.2.9 Score per residue for model 9

- Molecule 1: Trefoil factor 3

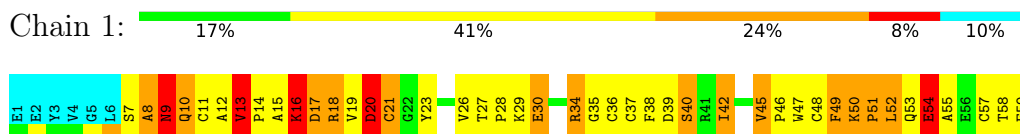


- Molecule 1: Trefoil factor 3

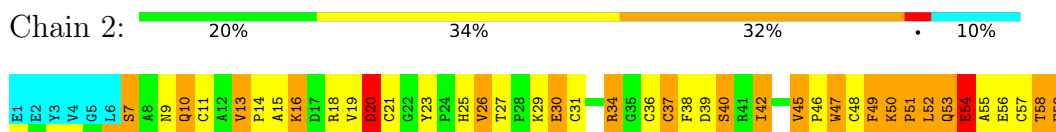


4.2.10 Score per residue for model 10

- Molecule 1: Trefoil factor 3

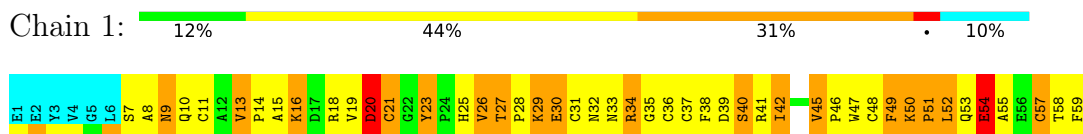


- Molecule 1: Trefoil factor 3

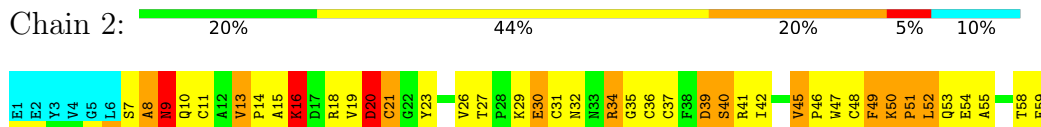


4.2.11 Score per residue for model 11

- Molecule 1: Trefoil factor 3

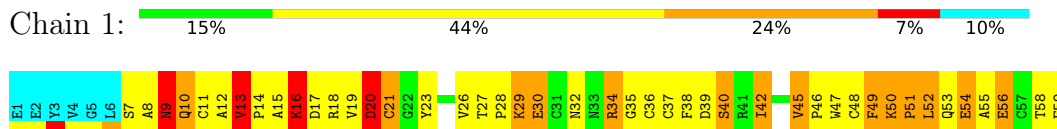


- Molecule 1: Trefoil factor 3

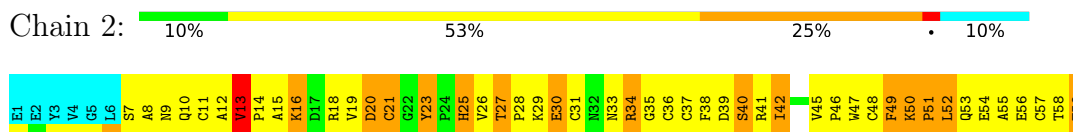


4.2.12 Score per residue for model 12

- Molecule 1: Trefoil factor 3

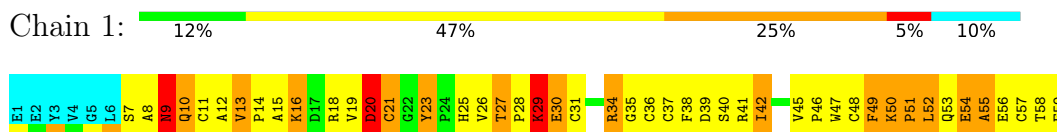


- Molecule 1: Trefoil factor 3

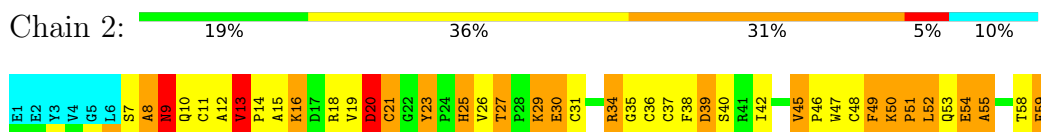


4.2.13 Score per residue for model 13

- Molecule 1: Trefoil factor 3

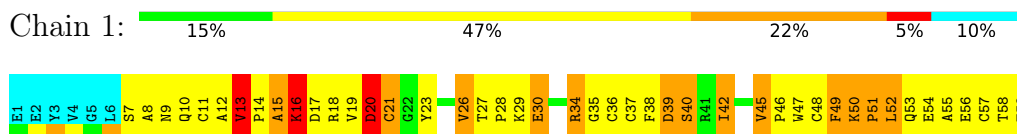


- Molecule 1: Trefoil factor 3

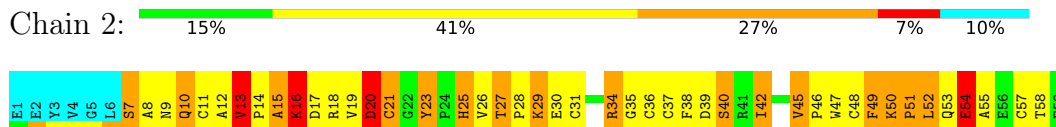


4.2.14 Score per residue for model 14

- Molecule 1: Trefoil factor 3

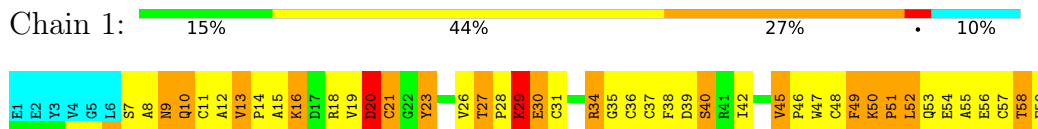


- Molecule 1: Trefoil factor 3

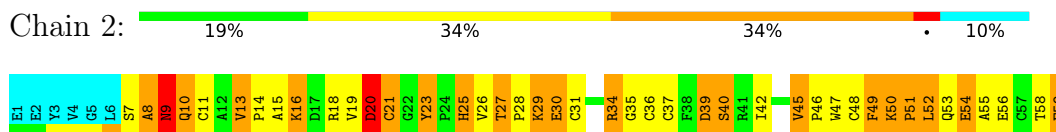


4.2.15 Score per residue for model 15

- Molecule 1: Trefoil factor 3

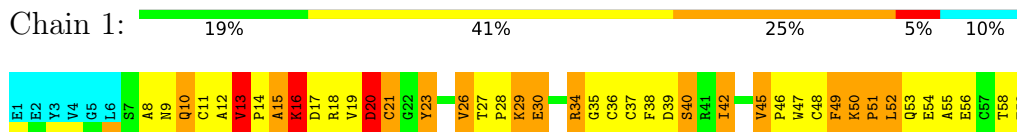


- Molecule 1: Trefoil factor 3

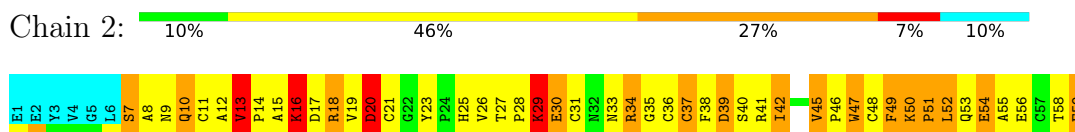


4.2.16 Score per residue for model 16

- Molecule 1: Trefoil factor 3

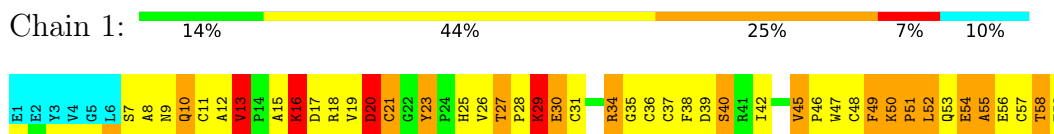


- Molecule 1: Trefoil factor 3

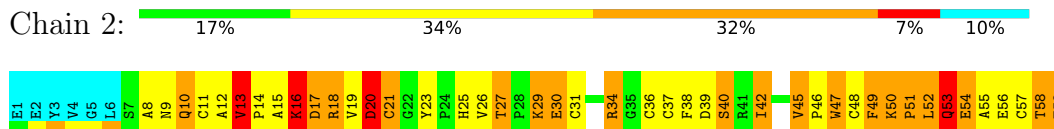


4.2.17 Score per residue for model 17

- Molecule 1: Trefoil factor 3

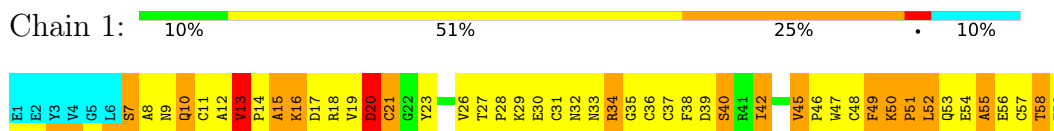


- Molecule 1: Trefoil factor 3

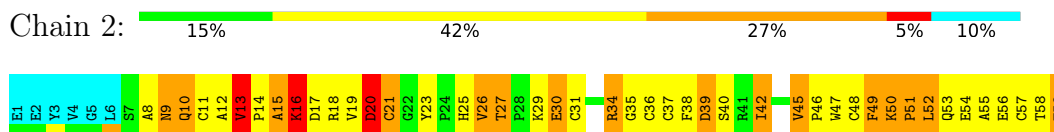


4.2.18 Score per residue for model 18

- Molecule 1: Trefoil factor 3

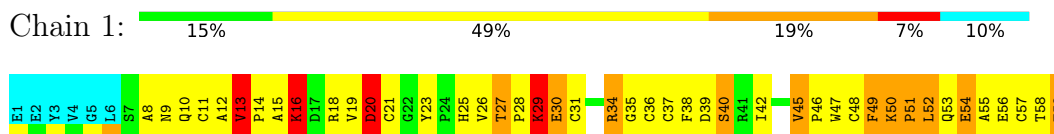


- Molecule 1: Trefoil factor 3

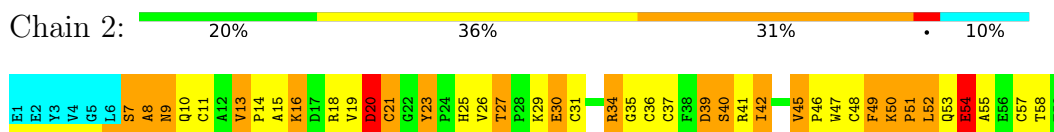


4.2.19 Score per residue for model 19

- Molecule 1: Trefoil factor 3

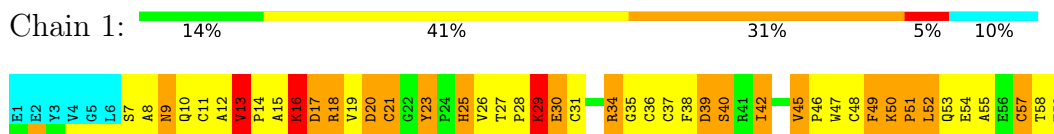


- Molecule 1: Trefoil factor 3

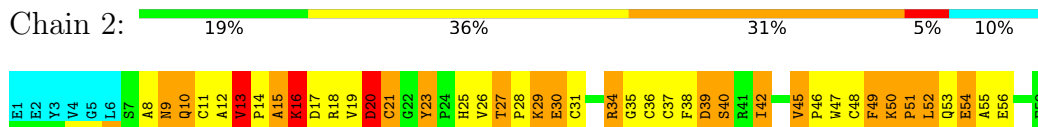


4.2.20 Score per residue for model 20

- Molecule 1: Trefoil factor 3

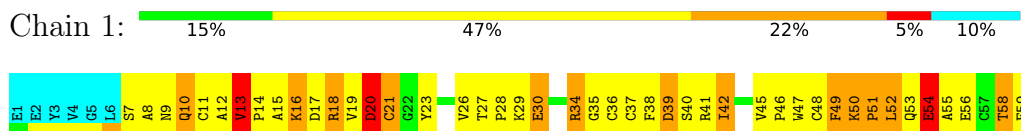


- Molecule 1: Trefoil factor 3

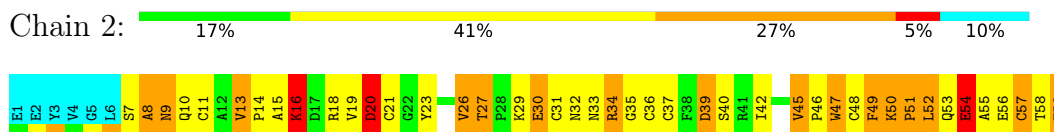


4.2.21 Score per residue for model 21

- Molecule 1: Trefoil factor 3

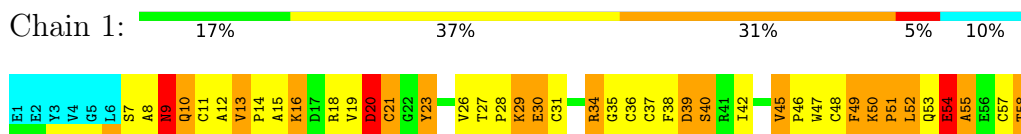


- Molecule 1: Trefoil factor 3

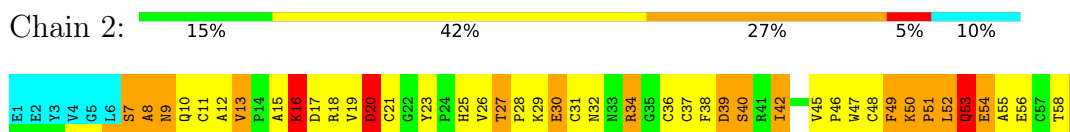


4.2.22 Score per residue for model 22

- Molecule 1: Trefoil factor 3

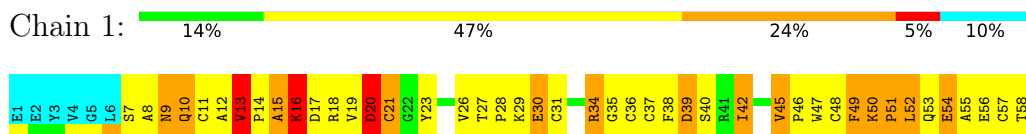


- Molecule 1: Trefoil factor 3

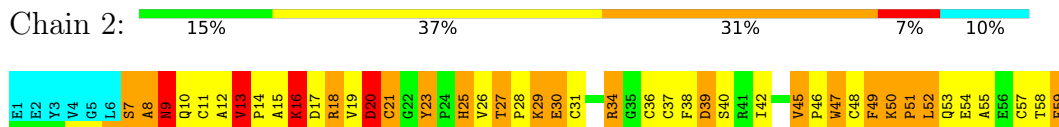


4.2.23 Score per residue for model 23

- Molecule 1: Trefoil factor 3

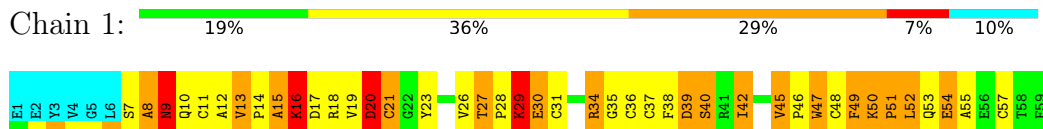


- Molecule 1: Trefoil factor 3

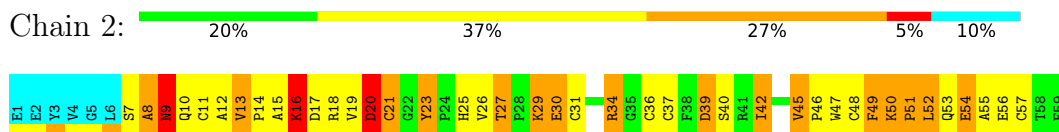


4.2.24 Score per residue for model 24

- Molecule 1: Trefoil factor 3

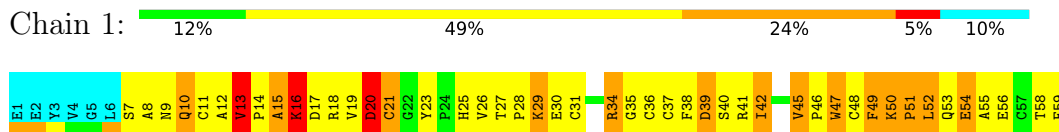


- Molecule 1: Trefoil factor 3

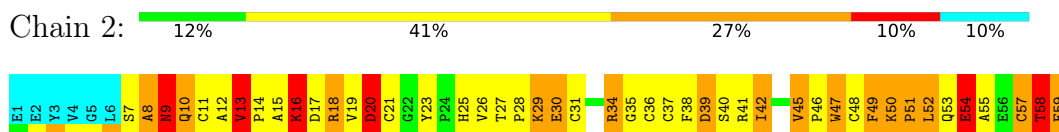


4.2.25 Score per residue for model 25

- Molecule 1: Trefoil factor 3

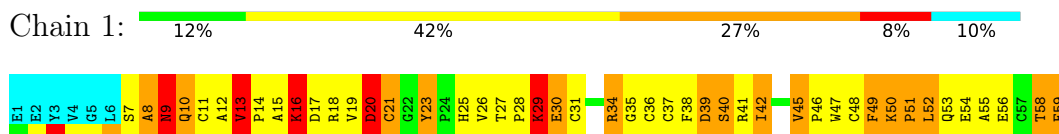


- Molecule 1: Trefoil factor 3

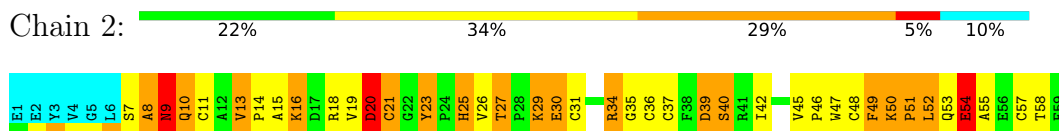


4.2.26 Score per residue for model 26

- Molecule 1: Trefoil factor 3

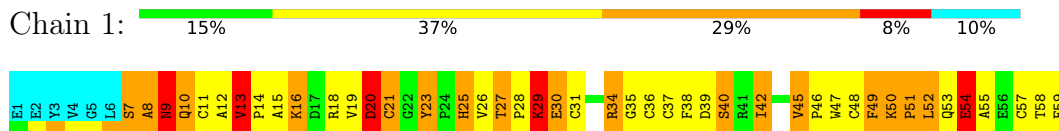


- Molecule 1: Trefoil factor 3

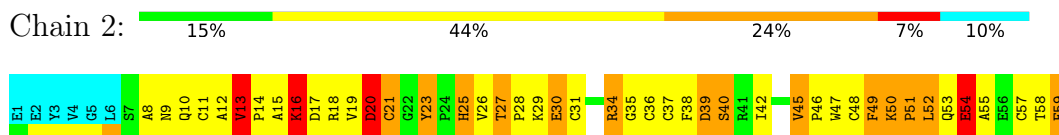


4.2.27 Score per residue for model 27

- Molecule 1: Trefoil factor 3

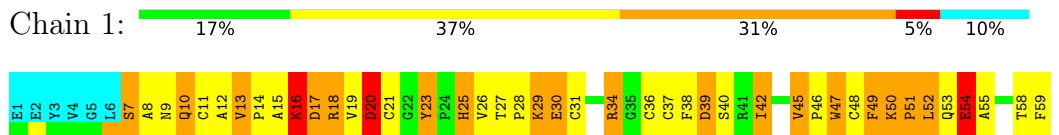


- Molecule 1: Trefoil factor 3

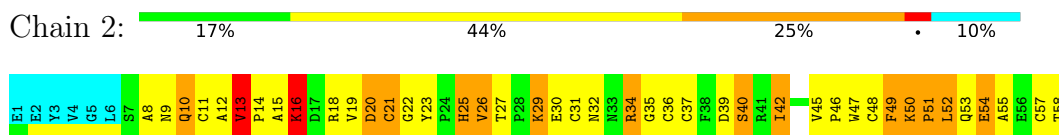


4.2.28 Score per residue for model 28

- Molecule 1: Trefoil factor 3



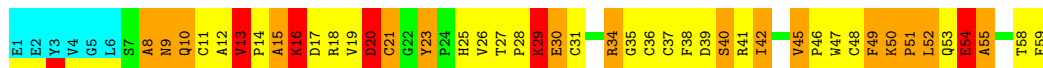
- Molecule 1: Trefoil factor 3



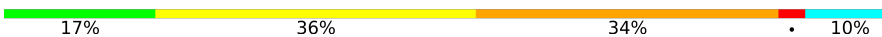
4.2.29 Score per residue for model 29

- Molecule 1: Trefoil factor 3

Chain 1: 



- Molecule 1: Trefoil factor 3

Chain 2: 



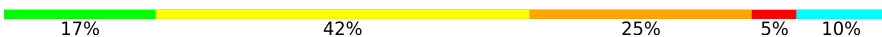
4.2.30 Score per residue for model 30

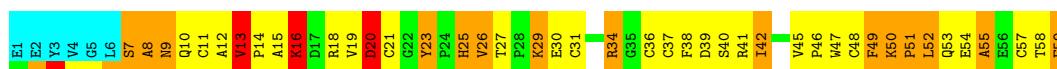
- Molecule 1: Trefoil factor 3

Chain 1: 



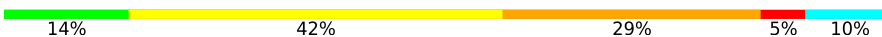
- Molecule 1: Trefoil factor 3

Chain 2: 



4.2.31 Score per residue for model 31

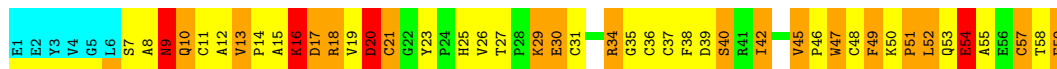
- Molecule 1: Trefoil factor 3

Chain 1: 



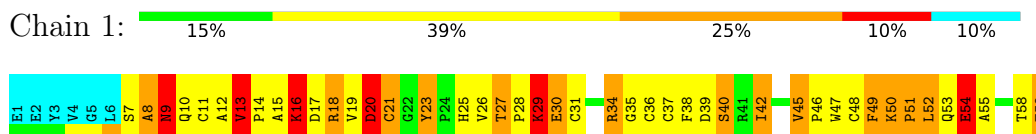
- Molecule 1: Trefoil factor 3

Chain 2: 

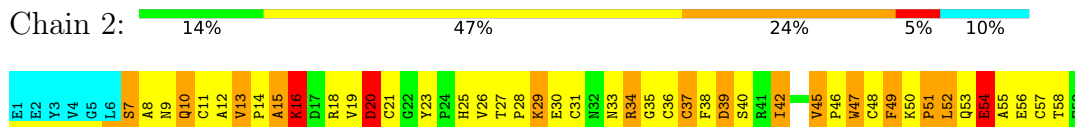


4.2.32 Score per residue for model 32

- Molecule 1: Trefoil factor 3

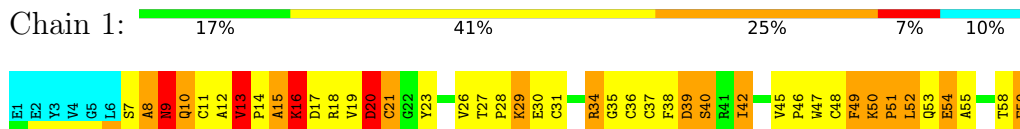


- Molecule 1: Trefoil factor 3

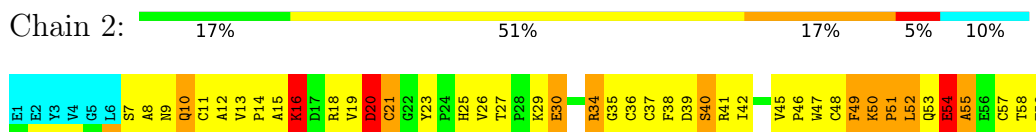


4.2.33 Score per residue for model 33

- Molecule 1: Trefoil factor 3

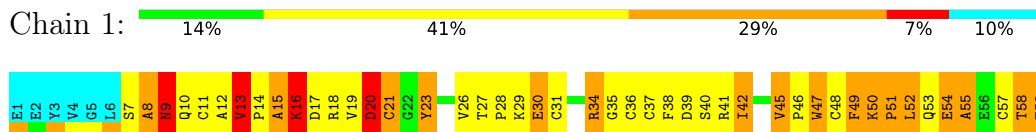


- Molecule 1: Trefoil factor 3

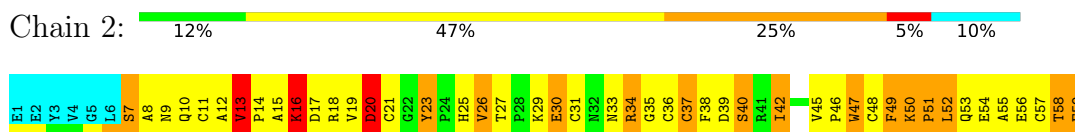


4.2.34 Score per residue for model 34

- Molecule 1: Trefoil factor 3

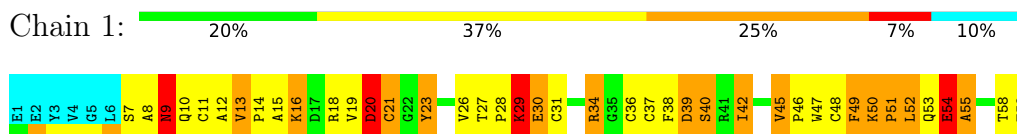


- Molecule 1: Trefoil factor 3

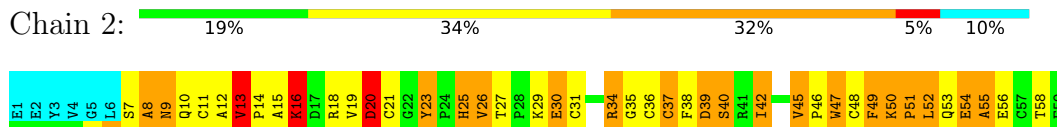


4.2.35 Score per residue for model 35

- Molecule 1: Trefoil factor 3

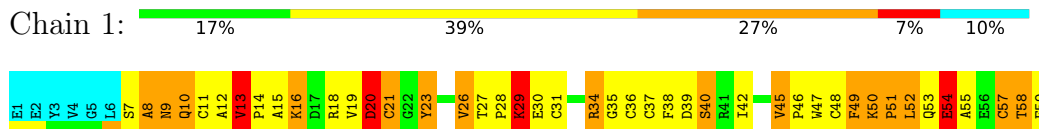


- Molecule 1: Trefoil factor 3

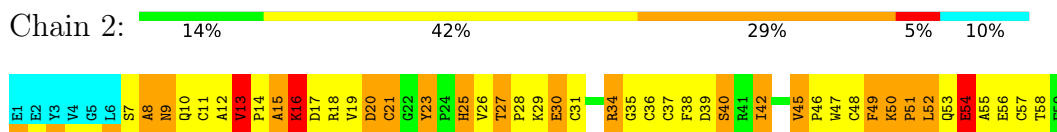


4.2.36 Score per residue for model 36

- Molecule 1: Trefoil factor 3

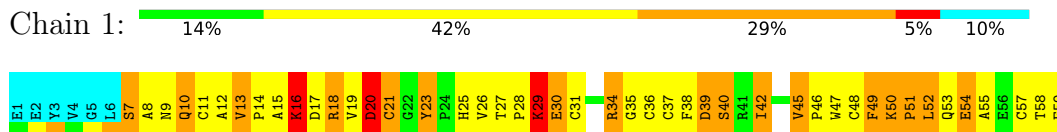


- Molecule 1: Trefoil factor 3

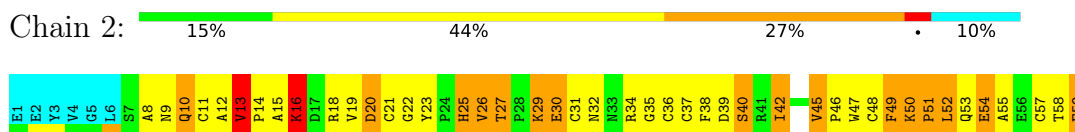


4.2.37 Score per residue for model 37

- Molecule 1: Trefoil factor 3

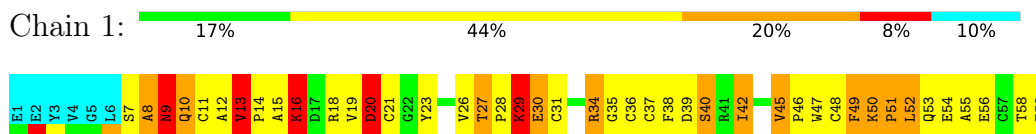


- Molecule 1: Trefoil factor 3

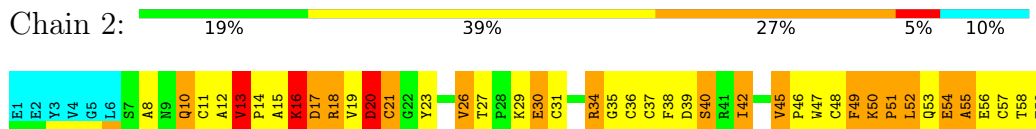


4.2.38 Score per residue for model 38

- Molecule 1: Trefoil factor 3

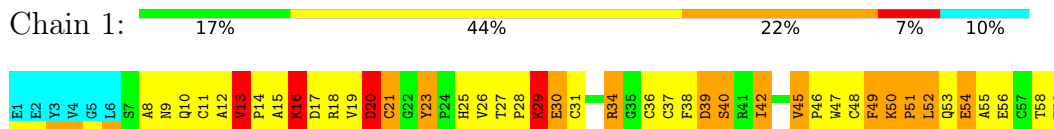


- Molecule 1: Trefoil factor 3

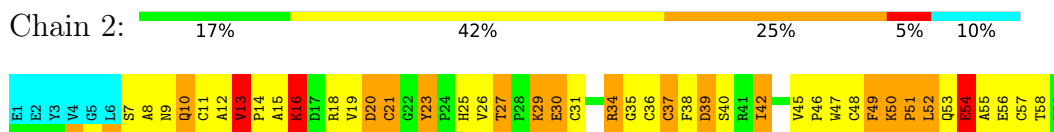


4.2.39 Score per residue for model 39 (medoid)

- Molecule 1: Trefoil factor 3

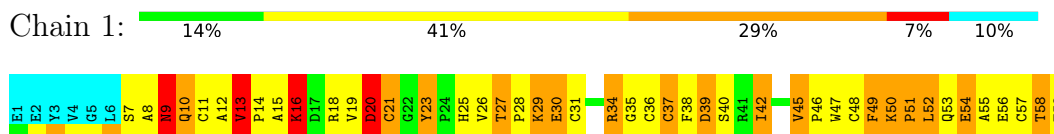


- Molecule 1: Trefoil factor 3

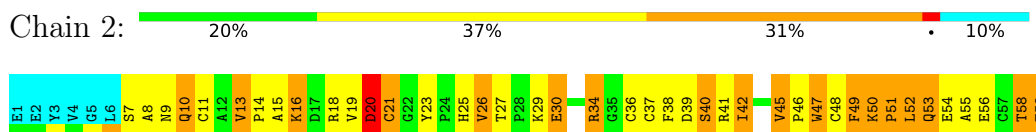


4.2.40 Score per residue for model 40

- Molecule 1: Trefoil factor 3

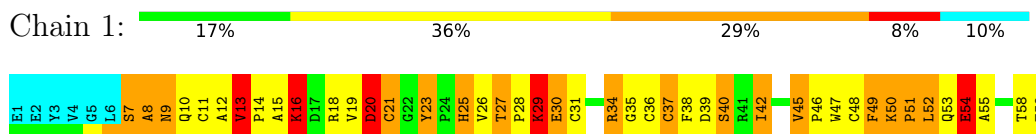


- Molecule 1: Trefoil factor 3

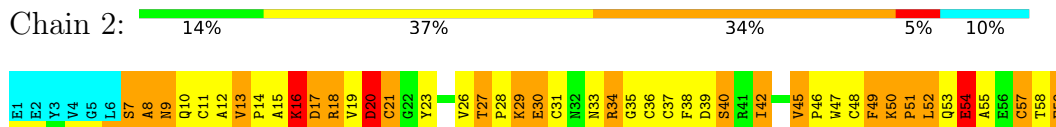


4.2.41 Score per residue for model 41

- Molecule 1: Trefoil factor 3

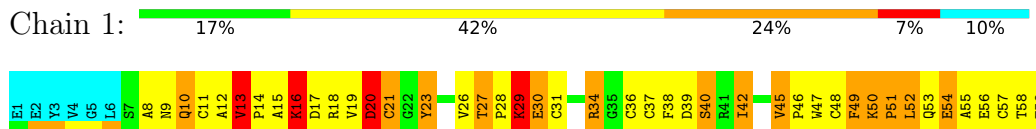


- Molecule 1: Trefoil factor 3

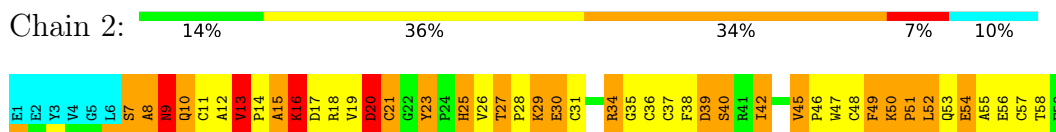


4.2.42 Score per residue for model 42

- Molecule 1: Trefoil factor 3

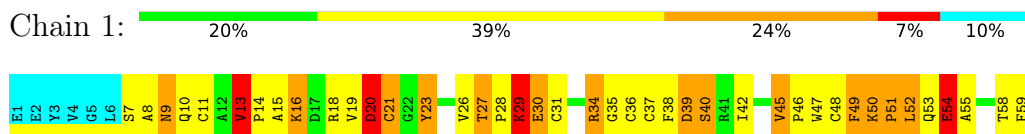


- Molecule 1: Trefoil factor 3

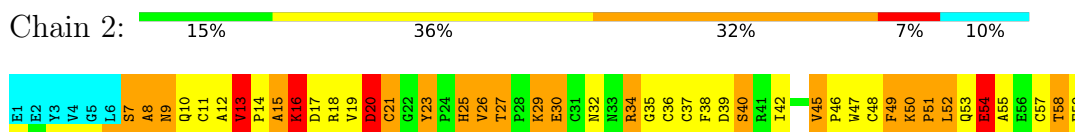


4.2.43 Score per residue for model 43

- Molecule 1: Trefoil factor 3



- Molecule 1: Trefoil factor 3



4.2.44 Score per residue for model 44

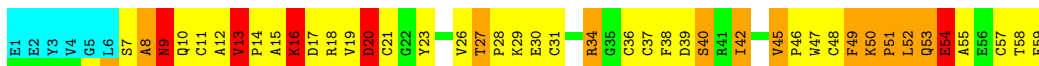
- Molecule 1: Trefoil factor 3

Chain 1: 15% 41% 27% 7% 10%



- Molecule 1: Trefoil factor 3

Chain 2: 17% 46% 19% 8% 10%



4.2.45 Score per residue for model 45

- Molecule 1: Trefoil factor 3

Chain 1: 10% 47% 25% 7% 10%



- Molecule 1: Trefoil factor 3

Chain 2: 15% 46% 25% 10%



4.2.46 Score per residue for model 46

- Molecule 1: Trefoil factor 3

Chain 1: 17% 46% 19% 8% 10%



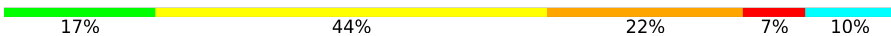
- Molecule 1: Trefoil factor 3

Chain 2: 19% 29% 36% 7% 10%



4.2.47 Score per residue for model 47

● Molecule 1: Trefoil factor 3

Chain 1:  17% 44% 22% 7% 10%

● Molecule 1: Trefoil factor 3

Chain 2:  19% 32% 34% 5% 10%

5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 47 were deposited, based on the following criterion: *structures with acceptable covalent geometry, structures with favorable non-bond energy, structures with the least restraint violations, structures with the lowest energy, target function*.

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

Software name	Classification	Version
DYANA	refinement	1.5

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts 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	1	408	377	376	74±7
1	2	408	377	376	72±7
All	All	38352	35438	35352	6753

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 92.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:1:15:ALA:HB1	1:1:45:VAL:HG21	1.07	1.25	4	29
1:2:15:ALA:HB1	1:2:45:VAL:HG21	1.00	1.32	47	35
1:1:15:ALA:CB	1:1:42:ILE:HD12	0.98	1.88	46	46
1:2:15:ALA:HB1	1:2:45:VAL:HG11	0.98	1.33	24	23
1:2:52:LEU:HD22	1:2:52:LEU:O	0.95	1.59	43	5
1:2:15:ALA:CB	1:2:42:ILE:HD12	0.95	1.92	8	46
1:1:7:SER:O	1:1:9:ASN:N	0.89	2.06	36	14
1:1:15:ALA:HB1	1:1:45:VAL:HG11	0.89	1.42	33	18
1:2:15:ALA:HB3	1:2:42:ILE:HD12	0.86	1.46	23	39
1:1:15:ALA:HB3	1:1:42:ILE:HD12	0.86	1.46	21	38
1:2:11:CYS:HB2	1:2:52:LEU:HD12	0.85	1.48	10	5
1:1:52:LEU:C	1:1:52:LEU:HD23	0.85	1.92	34	11
1:2:15:ALA:CB	1:2:45:VAL:HG21	0.84	2.03	47	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:1:13:VAL:HG22	1:1:14:PRO:HD2	0.84	1.48	4	30
1:2:52:LEU:C	1:2:52:LEU:HD13	0.84	1.93	10	4
1:2:13:VAL:HG22	1:2:14:PRO:HD2	0.83	1.51	29	35
1:2:7:SER:O	1:2:9:ASN:N	0.82	2.12	42	22
1:1:11:CYS:HB2	1:1:52:LEU:HD23	0.82	1.51	41	21
1:1:45:VAL:HG22	1:1:46:PRO:HD2	0.82	1.52	28	13
1:2:45:VAL:HG22	1:2:46:PRO:HD2	0.81	1.52	47	12
1:2:52:LEU:C	1:2:52:LEU:HD23	0.81	1.95	44	6
1:1:8:ALA:HA	1:1:52:LEU:HD12	0.81	1.53	47	11
1:2:8:ALA:HA	1:2:52:LEU:HD12	0.81	1.51	1	6
1:1:15:ALA:HB1	1:1:45:VAL:CG2	0.80	2.06	44	8
1:2:54:GLU:O	1:2:58:THR:HG22	0.79	1.77	30	8
1:2:11:CYS:HB2	1:2:52:LEU:HD23	0.79	1.54	29	13
1:2:15:ALA:HB1	1:2:45:VAL:CG2	0.78	2.07	47	5
1:2:11:CYS:CB	1:2:52:LEU:HD23	0.78	2.08	21	33
1:2:45:VAL:HG22	1:2:46:PRO:CD	0.78	2.09	23	12
1:1:18:ARG:CZ	1:1:49:PHE:CZ	0.78	2.67	41	23
1:1:15:ALA:CB	1:1:45:VAL:HG21	0.77	2.08	44	12
1:2:8:ALA:HA	1:2:52:LEU:HD22	0.77	1.54	21	34
1:2:8:ALA:O	1:2:9:ASN:CB	0.76	2.33	31	8
1:1:45:VAL:HG22	1:1:46:PRO:CD	0.76	2.11	28	13
1:2:18:ARG:CZ	1:2:49:PHE:CZ	0.75	2.69	34	31
1:1:11:CYS:SG	1:1:51:PRO:HG2	0.75	2.21	40	2
1:1:8:ALA:O	1:1:52:LEU:HD22	0.75	1.82	4	8
1:2:52:LEU:HD12	1:2:52:LEU:O	0.73	1.83	46	10
1:1:8:ALA:O	1:1:9:ASN:CB	0.73	2.37	9	10
1:1:11:CYS:CB	1:1:52:LEU:HD23	0.72	2.13	32	35
1:2:23:TYR:O	1:2:26:VAL:HG12	0.72	1.84	37	23
1:2:49:PHE:CD1	1:2:49:PHE:N	0.72	2.57	22	47
1:1:13:VAL:HG22	1:1:14:PRO:CD	0.72	2.14	19	30
1:2:10:GLN:CD	1:2:51:PRO:C	0.72	2.48	37	7
1:2:11:CYS:SG	1:2:51:PRO:HG2	0.72	2.25	29	5
1:2:13:VAL:HG22	1:2:14:PRO:CD	0.72	2.15	29	32
1:1:49:PHE:N	1:1:49:PHE:CD1	0.71	2.59	34	47
1:2:26:VAL:HG23	1:2:48:CYS:HB2	0.71	1.60	28	36
1:2:11:CYS:HB3	1:2:52:LEU:HD23	0.70	1.63	13	28
1:1:8:ALA:HA	1:1:52:LEU:HD13	0.70	1.63	32	32
1:2:21:CYS:SG	1:2:23:TYR:CD2	0.70	2.85	30	5
1:1:59:PHE:O	1:2:19:VAL:HG21	0.69	1.87	34	2
1:2:21:CYS:SG	1:2:23:TYR:CD1	0.69	2.86	37	4
1:2:10:GLN:NE2	1:2:51:PRO:HA	0.69	2.02	47	24

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:2:15:ALA:HB3	1:2:42:ILE:CD1	0.69	2.18	45	10
1:1:13:VAL:HG11	1:1:17:ASP:HB3	0.69	1.64	24	7
1:1:10:GLN:CD	1:1:51:PRO:C	0.68	2.51	40	15
1:2:18:ARG:NH1	1:2:49:PHE:CZ	0.68	2.62	32	4
1:1:23:TYR:CE1	1:1:34:ARG:CD	0.67	2.78	31	21
1:2:23:TYR:CE1	1:2:34:ARG:CD	0.67	2.78	46	17
1:2:13:VAL:HG13	1:2:14:PRO:HD2	0.67	1.65	33	2
1:1:21:CYS:N	1:1:48:CYS:O	0.67	2.28	44	47
1:2:18:ARG:NH1	1:2:49:PHE:CE1	0.66	2.63	32	12
1:2:11:CYS:CB	1:2:52:LEU:HD12	0.66	2.21	22	5
1:1:18:ARG:NH1	1:1:49:PHE:CZ	0.66	2.64	24	3
1:1:10:GLN:O	1:1:13:VAL:HG13	0.66	1.90	24	4
1:2:8:ALA:HA	1:2:52:LEU:HD13	0.66	1.68	9	32
1:2:14:PRO:O	1:2:15:ALA:HB3	0.66	1.90	32	8
1:1:18:ARG:NH1	1:1:49:PHE:CE1	0.65	2.63	24	15
1:2:21:CYS:N	1:2:48:CYS:O	0.65	2.27	47	47
1:2:52:LEU:HD23	1:2:52:LEU:O	0.65	1.92	1	6
1:2:21:CYS:SG	1:2:23:TYR:CE2	0.65	2.90	34	5
1:1:14:PRO:O	1:1:15:ALA:HB3	0.65	1.91	24	13
1:2:26:VAL:HG22	1:2:38:PHE:CE2	0.65	2.26	3	3
1:2:49:PHE:CD2	1:2:51:PRO:HG3	0.65	2.27	17	47
1:1:26:VAL:HG23	1:1:48:CYS:HB2	0.64	1.69	30	32
1:1:8:ALA:CA	1:1:52:LEU:HD13	0.64	2.23	32	18
1:2:15:ALA:CB	1:2:45:VAL:HG11	0.64	2.19	24	1
1:2:8:ALA:O	1:2:10:GLN:N	0.64	2.30	42	2
1:1:52:LEU:HD12	1:1:52:LEU:O	0.64	1.93	41	9
1:2:21:CYS:SG	1:2:23:TYR:CE1	0.64	2.91	22	5
1:2:54:GLU:HG2	1:2:58:THR:HG21	0.64	1.70	1	3
1:1:9:ASN:O	1:1:12:ALA:HB3	0.64	1.92	46	13
1:1:21:CYS:SG	1:1:23:TYR:CE1	0.64	2.91	38	5
1:1:23:TYR:OH	1:2:23:TYR:CE2	0.63	2.51	44	1
1:1:23:TYR:CE2	1:1:36:CYS:SG	0.63	2.92	45	2
1:2:8:ALA:CA	1:2:52:LEU:HD22	0.63	2.23	34	11
1:1:8:ALA:CA	1:1:52:LEU:HD12	0.63	2.24	47	3
1:1:21:CYS:SG	1:1:23:TYR:CD1	0.63	2.92	38	6
1:2:13:VAL:HG21	1:2:17:ASP:HB3	0.63	1.67	24	6
1:1:11:CYS:HB3	1:1:52:LEU:HD23	0.63	1.69	27	28
1:2:8:ALA:C	1:2:52:LEU:HD22	0.63	2.14	34	10
1:2:15:ALA:HB1	1:2:45:VAL:CG1	0.62	2.18	24	1
1:1:49:PHE:CE2	1:1:51:PRO:HG3	0.62	2.30	41	42
1:1:8:ALA:O	1:1:10:GLN:N	0.61	2.33	26	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:1:46:PRO:O	1:1:49:PHE:CE1	0.61	2.54	28	29
1:1:8:ALA:HA	1:1:52:LEU:HD22	0.61	1.70	33	30
1:2:19:VAL:HG12	1:2:19:VAL:O	0.61	1.95	40	4
1:1:11:CYS:HA	1:1:51:PRO:CB	0.61	2.26	1	45
1:2:11:CYS:HA	1:2:51:PRO:CB	0.61	2.25	23	42
1:2:39:ASP:O	1:2:40:SER:CB	0.61	2.49	23	47
1:1:8:ALA:C	1:1:52:LEU:HD22	0.61	2.16	37	7
1:1:10:GLN:HG3	1:1:11:CYS:N	0.61	2.11	18	4
1:2:55:ALA:O	1:2:59:PHE:CE1	0.61	2.54	40	2
1:1:18:ARG:NH1	1:1:45:VAL:CG2	0.61	2.63	34	29
1:1:15:ALA:CA	1:1:45:VAL:HG21	0.61	2.25	44	2
1:2:23:TYR:CE2	1:2:34:ARG:CD	0.61	2.84	8	2
1:2:46:PRO:O	1:2:49:PHE:CE1	0.60	2.54	47	39
1:2:52:LEU:O	1:2:52:LEU:HD13	0.60	1.97	32	3
1:1:52:LEU:C	1:1:52:LEU:CD2	0.60	2.69	43	10
1:1:23:TYR:CE1	1:1:34:ARG:HD2	0.60	2.32	31	21
1:1:8:ALA:O	1:1:9:ASN:HB2	0.60	1.97	35	3
1:1:10:GLN:NE2	1:1:51:PRO:HA	0.60	2.11	27	34
1:1:45:VAL:HG13	1:1:46:PRO:HD2	0.60	1.74	32	6
1:2:52:LEU:O	1:2:52:LEU:CD1	0.60	2.50	29	7
1:1:8:ALA:C	1:1:10:GLN:N	0.60	2.55	36	4
1:1:27:THR:C	1:1:38:PHE:CD1	0.60	2.75	45	3
1:2:36:CYS:HA	1:2:49:PHE:O	0.60	1.97	23	47
1:2:52:LEU:O	1:2:52:LEU:CD2	0.60	2.48	31	10
1:1:39:ASP:O	1:1:40:SER:CB	0.59	2.49	25	47
1:2:53:GLN:O	1:2:55:ALA:N	0.59	2.35	43	39
1:1:39:ASP:CG	1:1:40:SER:N	0.59	2.54	39	15
1:2:15:ALA:CA	1:2:45:VAL:HG21	0.59	2.27	47	3
1:1:15:ALA:HB2	1:1:42:ILE:HD12	0.59	1.74	46	1
1:2:39:ASP:CG	1:2:40:SER:N	0.59	2.55	22	26
1:2:8:ALA:O	1:2:11:CYS:N	0.59	2.35	21	1
1:1:23:TYR:CD2	1:1:36:CYS:SG	0.59	2.95	45	1
1:2:11:CYS:N	1:2:51:PRO:HB2	0.59	2.13	1	18
1:1:15:ALA:HB3	1:1:42:ILE:CD1	0.59	2.24	35	18
1:1:19:VAL:HG12	1:1:19:VAL:O	0.59	1.97	10	5
1:2:52:LEU:C	1:2:52:LEU:CD1	0.59	2.69	10	4
1:2:21:CYS:SG	1:2:23:TYR:CZ	0.59	2.95	44	2
1:1:45:VAL:CB	1:1:46:PRO:CD	0.59	2.79	21	34
1:2:8:ALA:CA	1:2:52:LEU:HD13	0.59	2.28	9	20
1:2:18:ARG:HG2	1:2:49:PHE:CD2	0.59	2.33	16	29
1:2:37:CYS:CB	1:2:51:PRO:CG	0.59	2.81	21	39

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:2:54:GLU:HA	1:2:58:THR:HG22	0.59	1.73	11	2
1:1:37:CYS:CB	1:1:51:PRO:CG	0.58	2.81	35	47
1:1:49:PHE:CD2	1:1:51:PRO:HG3	0.58	2.32	40	47
1:1:45:VAL:HB	1:1:46:PRO:CD	0.58	2.28	21	34
1:2:27:THR:HG22	1:2:30:GLU:H	0.58	1.58	27	27
1:2:15:ALA:CB	1:2:42:ILE:CD1	0.58	2.78	38	18
1:2:15:ALA:HB1	1:2:42:ILE:HD12	0.58	1.75	14	9
1:1:50:LYS:HA	1:1:53:GLN:CG	0.58	2.28	21	47
1:1:52:LEU:HD23	1:1:52:LEU:O	0.58	1.98	19	11
1:2:21:CYS:SG	1:2:50:LYS:CE	0.58	2.92	43	15
1:1:57:CYS:SG	1:1:58:THR:N	0.58	2.76	11	3
1:2:49:PHE:CE2	1:2:51:PRO:HG3	0.58	2.33	34	47
1:2:8:ALA:O	1:2:52:LEU:HD22	0.58	1.98	27	12
1:2:11:CYS:CA	1:2:51:PRO:HB2	0.58	2.28	1	37
1:1:9:ASN:ND2	1:1:12:ALA:HB3	0.58	2.13	36	1
1:2:23:TYR:CE2	1:2:34:ARG:CB	0.58	2.87	47	4
1:2:53:GLN:HE21	1:2:53:GLN:N	0.58	1.97	17	2
1:1:37:CYS:N	1:1:49:PHE:O	0.58	2.37	15	45
1:2:18:ARG:NH1	1:2:45:VAL:CG2	0.58	2.66	42	31
1:1:7:SER:O	1:1:8:ALA:C	0.58	2.42	26	7
1:2:45:VAL:CB	1:2:46:PRO:CD	0.57	2.82	22	35
1:2:18:ARG:NH1	1:2:45:VAL:CG1	0.57	2.67	43	10
1:2:45:VAL:HG13	1:2:46:PRO:HD2	0.57	1.74	16	9
1:1:23:TYR:CE2	1:1:34:ARG:CD	0.57	2.86	2	2
1:1:18:ARG:NH1	1:1:45:VAL:CG1	0.57	2.67	18	12
1:2:52:LEU:C	1:2:52:LEU:CD2	0.57	2.70	44	5
1:1:23:TYR:CE2	1:1:34:ARG:HD3	0.57	2.34	30	2
1:2:11:CYS:HB2	1:2:52:LEU:HD22	0.57	1.77	1	1
1:1:15:ALA:CB	1:1:42:ILE:CD1	0.57	2.81	38	23
1:2:53:GLN:NE2	1:2:54:GLU:N	0.56	2.52	40	3
1:1:15:ALA:HB1	1:1:42:ILE:HD12	0.56	1.75	29	8
1:2:21:CYS:CB	1:2:48:CYS:O	0.56	2.53	22	16
1:1:23:TYR:CE1	1:1:34:ARG:HD3	0.56	2.35	31	24
1:2:23:TYR:CE1	1:2:34:ARG:HD2	0.56	2.34	46	17
1:1:8:ALA:O	1:1:9:ASN:HB3	0.56	2.01	23	2
1:1:23:TYR:O	1:1:26:VAL:HG12	0.56	2.01	46	12
1:1:36:CYS:HA	1:1:49:PHE:O	0.56	2.00	40	46
1:1:19:VAL:O	1:1:20:ASP:C	0.56	2.43	39	47
1:2:54:GLU:O	1:2:55:ALA:C	0.56	2.44	33	47
1:1:39:ASP:OD2	1:1:42:ILE:O	0.56	2.24	44	4
1:2:45:VAL:HB	1:2:46:PRO:CD	0.56	2.30	39	35

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:1:10:GLN:OE1	1:1:51:PRO:O	0.56	2.23	33	3
1:1:45:VAL:HG13	1:1:46:PRO:CD	0.56	2.31	32	4
1:2:49:PHE:C	1:2:51:PRO:HD3	0.56	2.21	1	30
1:1:53:GLN:O	1:1:55:ALA:N	0.56	2.39	27	38
1:1:8:ALA:CB	1:1:52:LEU:HD13	0.56	2.31	44	4
1:1:23:TYR:CB	1:1:34:ARG:NH2	0.56	2.69	30	1
1:1:27:THR:HG22	1:1:30:GLU:H	0.55	1.61	40	19
1:2:37:CYS:N	1:2:49:PHE:O	0.55	2.39	43	43
1:1:18:ARG:NH1	1:1:45:VAL:HG23	0.55	2.15	3	28
1:1:10:GLN:CD	1:1:51:PRO:CA	0.55	2.75	37	4
1:1:34:ARG:CZ	1:1:36:CYS:SG	0.55	2.95	11	6
1:1:18:ARG:HG2	1:1:49:PHE:CD2	0.55	2.35	32	25
1:2:9:ASN:O	1:2:12:ALA:HB3	0.55	2.02	31	4
1:2:13:VAL:HG11	1:2:17:ASP:HB3	0.55	1.79	43	2
1:2:50:LYS:HA	1:2:53:GLN:CG	0.55	2.32	42	32
1:1:46:PRO:O	1:1:49:PHE:CD1	0.55	2.60	28	8
1:2:26:VAL:HG23	1:2:48:CYS:CB	0.55	2.32	28	2
1:1:8:ALA:CA	1:1:52:LEU:HD22	0.55	2.31	25	7
1:2:37:CYS:N	1:2:53:GLN:OE1	0.55	2.39	29	16
1:2:23:TYR:CE2	1:2:34:ARG:HD2	0.55	2.37	8	2
1:2:45:VAL:HG13	1:2:46:PRO:CD	0.55	2.32	16	4
1:2:46:PRO:O	1:2:49:PHE:CD1	0.55	2.60	47	7
1:1:18:ARG:NH1	1:1:45:VAL:HG13	0.55	2.17	1	8
1:2:39:ASP:OD2	1:2:42:ILE:O	0.55	2.25	16	5
1:2:7:SER:O	1:2:8:ALA:C	0.55	2.46	42	2
1:1:28:PRO:CD	1:1:38:PHE:CE1	0.55	2.90	24	3
1:1:34:ARG:NE	1:1:36:CYS:SG	0.54	2.80	34	17
1:2:35:GLY:C	1:2:53:GLN:NE2	0.54	2.61	46	26
1:1:45:VAL:HB	1:1:46:PRO:HD2	0.54	1.80	2	34
1:2:23:TYR:CE1	1:2:34:ARG:HD3	0.54	2.36	14	17
1:2:38:PHE:CD1	1:2:47:TRP:O	0.54	2.60	34	4
1:2:18:ARG:NH1	1:2:45:VAL:HG23	0.54	2.17	18	29
1:1:8:ALA:C	1:1:10:GLN:H	0.54	2.05	36	1
1:2:45:VAL:HB	1:2:46:PRO:HD2	0.54	1.78	30	35
1:1:21:CYS:CB	1:1:48:CYS:O	0.54	2.55	28	9
1:1:54:GLU:HG2	1:1:58:THR:HG22	0.54	1.79	21	1
1:2:8:ALA:C	1:2:10:GLN:N	0.54	2.57	42	2
1:1:28:PRO:O	1:1:29:LYS:HB2	0.54	2.03	45	35
1:1:54:GLU:O	1:1:58:THR:HG22	0.54	2.02	44	3
1:1:59:PHE:CG	1:1:59:PHE:O	0.54	2.60	36	1
1:1:30:GLU:O	1:1:33:ASN:HB3	0.54	2.03	45	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:2:18:ARG:NH1	1:2:45:VAL:HG13	0.54	2.18	14	7
1:2:36:CYS:CA	1:2:49:PHE:O	0.54	2.56	5	37
1:2:11:CYS:CA	1:2:51:PRO:CB	0.54	2.85	1	23
1:2:19:VAL:O	1:2:20:ASP:C	0.54	2.46	3	47
1:2:36:CYS:C	1:2:53:GLN:OE1	0.54	2.47	30	41
1:1:27:THR:HG21	1:1:30:GLU:OE1	0.54	2.02	2	1
1:1:28:PRO:HB3	1:1:38:PHE:CD2	0.53	2.38	38	34
1:1:28:PRO:N	1:1:38:PHE:CE1	0.53	2.76	24	2
1:1:23:TYR:CG	1:1:34:ARG:NE	0.53	2.76	30	1
1:2:34:ARG:NE	1:2:36:CYS:SG	0.53	2.81	25	19
1:1:55:ALA:O	1:1:59:PHE:CD1	0.53	2.61	34	1
1:2:52:LEU:O	1:2:52:LEU:CG	0.53	2.56	46	33
1:2:45:VAL:CG2	1:2:46:PRO:HD2	0.53	2.32	38	15
1:2:14:PRO:O	1:2:15:ALA:CB	0.53	2.55	32	8
1:1:12:ALA:O	1:1:13:VAL:O	0.53	2.26	16	36
1:1:36:CYS:CA	1:1:49:PHE:O	0.53	2.56	47	37
1:1:45:VAL:CG2	1:1:46:PRO:HD2	0.53	2.31	44	22
1:2:15:ALA:C	1:2:16:LYS:CG	0.53	2.76	47	30
1:2:18:ARG:NH1	1:2:46:PRO:O	0.53	2.42	30	37
1:1:36:CYS:CA	1:1:53:GLN:OE1	0.53	2.56	40	1
1:1:14:PRO:O	1:1:15:ALA:CB	0.53	2.57	18	13
1:2:23:TYR:CE2	1:2:34:ARG:HB3	0.53	2.39	1	2
1:1:30:GLU:O	1:1:34:ARG:CG	0.53	2.57	44	21
1:1:15:ALA:O	1:1:16:LYS:CB	0.53	2.56	28	21
1:2:53:GLN:N	1:2:53:GLN:NE2	0.53	2.55	8	2
1:1:15:ALA:C	1:1:16:LYS:CG	0.53	2.77	40	32
1:1:53:GLN:O	1:1:57:CYS:CB	0.53	2.57	22	5
1:2:25:HIS:CD2	1:2:30:GLU:OE2	0.53	2.61	6	1
1:2:15:ALA:O	1:2:16:LYS:CB	0.53	2.57	38	26
1:1:38:PHE:CE2	1:1:40:SER:HB2	0.53	2.39	9	29
1:1:23:TYR:CD2	1:1:34:ARG:HD2	0.52	2.38	26	4
1:1:37:CYS:O	1:1:49:PHE:CE1	0.52	2.62	24	3
1:2:37:CYS:HB2	1:2:51:PRO:CD	0.52	2.34	16	31
1:2:26:VAL:HA	1:2:31:CYS:SG	0.52	2.45	25	44
1:2:8:ALA:O	1:2:9:ASN:HB2	0.52	2.02	31	2
1:1:30:GLU:O	1:1:34:ARG:N	0.52	2.42	11	37
1:2:10:GLN:NE2	1:2:51:PRO:O	0.52	2.43	47	15
1:2:36:CYS:CB	1:2:48:CYS:SG	0.52	2.98	45	12
1:2:10:GLN:NE2	1:2:51:PRO:C	0.52	2.63	21	6
1:1:34:ARG:CZ	1:2:34:ARG:O	0.52	2.58	11	3
1:1:18:ARG:NH1	1:1:46:PRO:O	0.52	2.42	14	40

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:2:10:GLN:HE21	1:2:51:PRO:C	0.52	2.07	1	4
1:1:52:LEU:O	1:1:52:LEU:CG	0.52	2.57	40	12
1:1:35:GLY:C	1:1:53:GLN:NE2	0.52	2.63	21	14
1:2:19:VAL:O	1:2:19:VAL:HG12	0.52	2.04	13	13
1:2:28:PRO:HD3	1:2:38:PHE:CZ	0.52	2.39	16	4
1:1:34:ARG:CZ	1:2:33:ASN:O	0.52	2.58	8	1
1:1:28:PRO:HB3	1:1:38:PHE:CD1	0.52	2.40	30	1
1:2:11:CYS:SG	1:2:52:LEU:HD23	0.52	2.44	34	2
1:1:36:CYS:CB	1:1:48:CYS:SG	0.52	2.98	11	9
1:1:10:GLN:CD	1:1:51:PRO:HA	0.52	2.25	27	6
1:2:53:GLN:C	1:2:55:ALA:N	0.52	2.64	43	44
1:1:26:VAL:HA	1:1:31:CYS:SG	0.51	2.45	46	38
1:1:57:CYS:O	1:2:50:LYS:CB	0.51	2.58	36	13
1:1:18:ARG:HB3	1:1:49:PHE:CB	0.51	2.35	6	36
1:2:18:ARG:HB3	1:2:49:PHE:CB	0.51	2.35	43	34
1:1:28:PRO:HB3	1:1:38:PHE:CE2	0.51	2.40	46	24
1:1:23:TYR:OH	1:2:23:TYR:CZ	0.51	2.64	44	1
1:2:30:GLU:O	1:2:34:ARG:CG	0.51	2.59	19	16
1:1:21:CYS:SG	1:1:50:LYS:CE	0.51	2.99	37	13
1:2:10:GLN:CD	1:2:51:PRO:O	0.51	2.48	37	3
1:1:7:SER:O	1:1:52:LEU:CB	0.51	2.59	17	8
1:1:19:VAL:O	1:1:19:VAL:HG12	0.51	2.04	5	7
1:2:36:CYS:SG	1:2:50:LYS:CE	0.51	2.99	35	6
1:2:7:SER:O	1:2:10:GLN:HB2	0.51	2.06	46	4
1:2:21:CYS:SG	1:2:34:ARG:CZ	0.51	2.99	10	2
1:1:13:VAL:HG21	1:1:17:ASP:HB3	0.51	1.82	47	7
1:2:58:THR:CG2	1:2:59:PHE:N	0.51	2.74	41	4
1:1:52:LEU:O	1:1:52:LEU:CD1	0.51	2.58	40	2
1:1:30:GLU:O	1:1:34:ARG:HD3	0.51	2.06	45	1
1:2:12:ALA:O	1:2:13:VAL:O	0.51	2.29	42	36
1:2:8:ALA:HA	1:2:52:LEU:HD23	0.51	1.83	32	2
1:1:21:CYS:SG	1:1:34:ARG:CZ	0.51	2.99	24	5
1:1:10:GLN:CD	1:1:51:PRO:O	0.51	2.49	35	11
1:1:34:ARG:NH1	1:2:34:ARG:NH1	0.51	2.59	43	1
1:1:45:VAL:CB	1:1:46:PRO:HD2	0.51	2.35	21	32
1:2:23:TYR:CD1	1:2:34:ARG:HD2	0.51	2.41	42	17
1:1:23:TYR:CE2	1:1:34:ARG:HG3	0.51	2.41	45	1
1:2:37:CYS:CB	1:2:51:PRO:HG2	0.51	2.36	1	12
1:2:36:CYS:CA	1:2:53:GLN:OE1	0.50	2.59	13	5
1:1:54:GLU:O	1:1:58:THR:CG2	0.50	2.59	44	2
1:1:11:CYS:SG	1:1:52:LEU:HD23	0.50	2.45	40	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:2:38:PHE:CE2	1:2:40:SER:HB2	0.50	2.42	37	17
1:1:39:ASP:OD1	1:1:41:ARG:N	0.50	2.44	45	3
1:1:26:VAL:HG23	1:1:31:CYS:SG	0.50	2.47	15	8
1:2:21:CYS:SG	1:2:50:LYS:CD	0.50	2.99	23	6
1:2:23:TYR:CD2	1:2:34:ARG:HD2	0.50	2.42	43	2
1:1:10:GLN:NE2	1:1:51:PRO:O	0.50	2.44	44	24
1:1:28:PRO:HD3	1:1:38:PHE:CZ	0.50	2.42	45	18
1:1:23:TYR:CD1	1:1:34:ARG:HD2	0.50	2.42	37	20
1:2:21:CYS:SG	1:2:50:LYS:HE3	0.50	2.47	5	20
1:2:28:PRO:HB3	1:2:38:PHE:CD2	0.50	2.42	32	16
1:2:50:LYS:O	1:2:53:GLN:OE1	0.50	2.29	17	2
1:1:50:LYS:CE	1:2:56:GLU:O	0.50	2.59	34	3
1:2:7:SER:O	1:2:52:LEU:CB	0.50	2.59	10	6
1:1:31:CYS:O	1:1:36:CYS:N	0.50	2.36	45	1
1:2:13:VAL:CG2	1:2:14:PRO:HD2	0.50	2.34	46	20
1:2:34:ARG:CD	1:2:34:ARG:C	0.50	2.79	38	14
1:2:52:LEU:HD13	1:2:52:LEU:O	0.50	2.07	10	1
1:2:30:GLU:O	1:2:34:ARG:N	0.50	2.44	45	30
1:1:34:ARG:CD	1:1:34:ARG:C	0.49	2.80	16	11
1:1:13:VAL:CG2	1:1:14:PRO:HD2	0.49	2.33	19	18
1:1:21:CYS:SG	1:1:50:LYS:HE3	0.49	2.48	39	25
1:2:14:PRO:O	1:2:16:LYS:CG	0.49	2.60	35	9
1:1:12:ALA:O	1:1:13:VAL:C	0.49	2.51	46	7
1:1:58:THR:O	1:1:59:PHE:C	0.49	2.51	34	46
1:1:59:PHE:O	1:1:59:PHE:CD2	0.49	2.65	36	1
1:1:30:GLU:C	1:1:34:ARG:HD3	0.49	2.27	45	1
1:2:23:TYR:CE2	1:2:36:CYS:SG	0.49	3.06	1	2
1:2:37:CYS:HB2	1:2:51:PRO:CG	0.49	2.37	47	27
1:1:56:GLU:O	1:2:50:LYS:NZ	0.49	2.45	14	10
1:1:11:CYS:CA	1:1:51:PRO:HB2	0.49	2.37	27	32
1:1:23:TYR:CE2	1:1:34:ARG:HD2	0.49	2.42	2	2
1:2:8:ALA:O	1:2:9:ASN:HB3	0.49	2.07	31	1
1:1:14:PRO:O	1:1:16:LYS:CG	0.49	2.60	40	3
1:1:54:GLU:O	1:1:58:THR:CB	0.49	2.61	44	2
1:2:58:THR:O	1:2:59:PHE:C	0.49	2.51	16	26
1:1:10:GLN:NE2	1:2:59:PHE:C	0.49	2.66	18	9
1:2:26:VAL:HG21	1:2:47:TRP:HE3	0.49	1.68	3	9
1:2:26:VAL:HG22	1:2:38:PHE:HE2	0.49	1.67	3	3
1:2:26:VAL:CG2	1:2:38:PHE:CE2	0.49	2.96	3	2
1:1:28:PRO:HD3	1:1:38:PHE:CE1	0.49	2.43	24	3
1:1:10:GLN:OE1	1:1:51:PRO:C	0.49	2.51	33	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:2:45:VAL:HG13	1:2:46:PRO:N	0.49	2.23	16	11
1:2:18:ARG:NH1	1:2:45:VAL:HG11	0.49	2.23	23	3
1:2:8:ALA:HA	1:2:52:LEU:CD1	0.49	2.34	1	8
1:1:50:LYS:HA	1:1:53:GLN:HG3	0.49	1.85	38	29
1:1:45:VAL:HG13	1:1:46:PRO:N	0.49	2.22	31	8
1:2:18:ARG:NE	1:2:49:PHE:CZ	0.49	2.80	34	1
1:2:45:VAL:CB	1:2:46:PRO:HD2	0.49	2.38	2	35
1:2:54:GLU:CA	1:2:58:THR:HG22	0.49	2.37	11	2
1:2:19:VAL:O	1:2:20:ASP:O	0.48	2.31	31	20
1:1:10:GLN:NE2	1:1:51:PRO:C	0.48	2.67	30	17
1:1:53:GLN:C	1:1:55:ALA:N	0.48	2.65	27	47
1:2:21:CYS:SG	1:2:50:LYS:NZ	0.48	2.85	47	2
1:2:42:ILE:CG2	1:2:45:VAL:HG13	0.48	2.38	45	5
1:2:11:CYS:CB	1:2:52:LEU:CD2	0.48	2.89	21	1
1:1:23:TYR:HB3	1:1:34:ARG:NH2	0.48	2.23	30	1
1:2:39:ASP:OD2	1:2:40:SER:N	0.48	2.46	45	8
1:2:50:LYS:HB2	1:2:53:GLN:OE1	0.48	2.09	8	2
1:2:51:PRO:O	1:2:53:GLN:OE1	0.48	2.32	44	4
1:2:9:ASN:ND2	1:2:12:ALA:HB3	0.48	2.23	32	1
1:2:53:GLN:N	1:2:53:GLN:CD	0.48	2.66	22	2
1:2:34:ARG:CZ	1:2:36:CYS:SG	0.48	3.02	21	2
1:1:11:CYS:CA	1:1:51:PRO:CB	0.48	2.92	27	20
1:1:36:CYS:C	1:1:53:GLN:OE1	0.48	2.52	5	29
1:2:52:LEU:C	1:2:54:GLU:N	0.48	2.66	17	29
1:1:28:PRO:HG3	1:1:38:PHE:CE2	0.48	2.44	10	5
1:1:21:CYS:SG	1:1:50:LYS:CD	0.48	3.02	35	8
1:2:27:THR:HG22	1:2:30:GLU:N	0.48	2.24	27	8
1:2:11:CYS:HB2	1:2:51:PRO:HG2	0.48	1.85	43	1
1:1:19:VAL:O	1:1:20:ASP:O	0.48	2.32	10	31
1:1:8:ALA:O	1:1:52:LEU:CD2	0.48	2.59	18	3
1:1:15:ALA:CB	1:1:45:VAL:HG11	0.48	2.33	26	1
1:1:51:PRO:O	1:2:58:THR:O	0.47	2.31	38	17
1:2:25:HIS:O	1:2:26:VAL:C	0.47	2.53	19	23
1:1:45:VAL:CG2	1:1:46:PRO:CD	0.47	2.90	44	10
1:2:28:PRO:CD	1:2:38:PHE:CE1	0.47	2.97	23	1
1:1:8:ALA:O	1:1:11:CYS:N	0.47	2.45	26	2
1:1:27:THR:HG23	1:1:28:PRO:HD2	0.47	1.86	13	3
1:2:53:GLN:CD	1:2:53:GLN:N	0.47	2.67	40	2
1:1:54:GLU:O	1:1:55:ALA:C	0.47	2.51	41	34
1:1:54:GLU:CB	1:2:58:THR:OG1	0.47	2.62	40	8
1:1:15:ALA:O	1:1:16:LYS:CG	0.47	2.63	40	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:2:52:LEU:O	1:2:54:GLU:N	0.47	2.47	8	5
1:1:57:CYS:O	1:1:58:THR:C	0.47	2.51	15	2
1:2:45:VAL:CG2	1:2:46:PRO:CD	0.47	2.89	23	10
1:2:28:PRO:HB3	1:2:38:PHE:CE2	0.47	2.45	23	1
1:2:35:GLY:C	1:2:53:GLN:OE1	0.47	2.53	9	9
1:1:42:ILE:HB	1:1:45:VAL:HG13	0.47	1.86	10	2
1:1:34:ARG:NH1	1:2:33:ASN:O	0.47	2.47	34	4
1:1:34:ARG:O	1:2:34:ARG:NH1	0.47	2.48	16	5
1:1:57:CYS:O	1:1:59:PHE:N	0.47	2.48	15	2
1:2:35:GLY:O	1:2:53:GLN:NE2	0.47	2.48	28	4
1:2:26:VAL:HG22	1:2:38:PHE:HE1	0.47	1.68	29	1
1:1:58:THR:CG2	1:1:59:PHE:N	0.47	2.78	7	3
1:1:36:CYS:O	1:1:53:GLN:OE1	0.47	2.33	13	19
1:2:51:PRO:HD2	1:2:53:GLN:OE1	0.47	2.09	4	9
1:1:7:SER:C	1:1:52:LEU:HB2	0.47	2.30	22	4
1:1:37:CYS:HB2	1:1:51:PRO:CG	0.47	2.39	41	34
1:1:39:ASP:CB	1:1:47:TRP:HA	0.47	2.39	24	4
1:2:34:ARG:CD	1:2:36:CYS:SG	0.47	3.03	3	13
1:1:59:PHE:CE1	1:2:50:LYS:HG3	0.47	2.45	7	1
1:1:34:ARG:CD	1:1:36:CYS:SG	0.46	3.03	33	7
1:1:37:CYS:HB3	1:1:51:PRO:CG	0.46	2.41	47	11
1:2:17:ASP:O	1:2:18:ARG:O	0.46	2.33	25	8
1:1:58:THR:O	1:2:53:GLN:NE2	0.46	2.48	17	1
1:1:21:CYS:HB2	1:1:48:CYS:O	0.46	2.10	28	5
1:2:23:TYR:O	1:2:26:VAL:CG1	0.46	2.60	37	3
1:1:26:VAL:HA	1:1:34:ARG:NH2	0.46	2.26	30	1
1:1:30:GLU:O	1:1:34:ARG:CD	0.46	2.63	45	1
1:1:49:PHE:C	1:1:51:PRO:HD3	0.46	2.30	41	36
1:1:10:GLN:NE2	1:2:59:PHE:O	0.46	2.44	40	7
1:1:7:SER:O	1:1:52:LEU:HB3	0.46	2.10	17	10
1:2:27:THR:HG23	1:2:28:PRO:HD2	0.46	1.88	20	6
1:1:25:HIS:O	1:1:26:VAL:C	0.46	2.54	9	10
1:2:27:THR:C	1:2:38:PHE:CD2	0.46	2.89	13	2
1:1:39:ASP:OD2	1:1:40:SER:N	0.46	2.48	35	6
1:2:28:PRO:HD3	1:2:38:PHE:CE1	0.46	2.45	23	3
1:1:39:ASP:HB3	1:1:47:TRP:HA	0.46	1.87	25	3
1:1:13:VAL:HG23	1:1:14:PRO:HD2	0.46	1.87	46	1
1:1:13:VAL:CG1	1:1:17:ASP:HB3	0.46	2.38	24	13
1:2:53:GLN:O	1:2:54:GLU:C	0.46	2.53	43	13
1:2:27:THR:HA	1:2:38:PHE:CE1	0.46	2.45	18	3
1:2:14:PRO:O	1:2:16:LYS:HG2	0.46	2.10	47	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:2:19:VAL:O	1:2:19:VAL:CG1	0.46	2.63	40	2
1:1:52:LEU:O	1:1:52:LEU:CD2	0.46	2.63	11	8
1:1:30:GLU:O	1:1:34:ARG:HG2	0.46	2.09	44	16
1:1:27:THR:HA	1:1:38:PHE:CE1	0.46	2.46	3	2
1:2:35:GLY:O	1:2:53:GLN:HG3	0.46	2.10	46	10
1:1:9:ASN:O	1:1:9:ASN:ND2	0.46	2.48	35	1
1:1:37:CYS:HB2	1:1:51:PRO:CD	0.46	2.41	28	45
1:1:8:ALA:HA	1:1:52:LEU:CD1	0.46	2.35	19	16
1:2:8:ALA:O	1:2:9:ASN:C	0.46	2.53	21	2
1:1:45:VAL:HG23	1:1:46:PRO:HD2	0.46	1.87	37	2
1:1:23:TYR:CD1	1:1:34:ARG:NH2	0.46	2.83	45	1
1:1:7:SER:O	1:1:10:GLN:HB3	0.46	2.11	40	4
1:2:37:CYS:HB3	1:2:51:PRO:CG	0.46	2.41	37	8
1:1:34:ARG:NH1	1:2:34:ARG:O	0.45	2.49	14	9
1:1:10:GLN:OE1	1:1:51:PRO:CB	0.45	2.65	4	3
1:1:27:THR:HG22	1:1:30:GLU:N	0.45	2.25	40	3
1:2:52:LEU:O	1:2:52:LEU:HD12	0.45	2.11	18	5
1:1:38:PHE:CE2	1:1:40:SER:HB3	0.45	2.46	47	1
1:1:35:GLY:C	1:1:53:GLN:OE1	0.45	2.54	37	26
1:2:26:VAL:HG23	1:2:47:TRP:O	0.45	2.11	25	2
1:1:18:ARG:NH1	1:1:45:VAL:HG11	0.45	2.26	28	1
1:1:28:PRO:O	1:1:29:LYS:CB	0.45	2.62	45	1
1:1:50:LYS:HA	1:1:53:GLN:HG2	0.45	1.88	43	9
1:2:36:CYS:HB2	1:2:48:CYS:SG	0.45	2.52	1	1
1:2:27:THR:HA	1:2:38:PHE:CE2	0.45	2.46	17	2
1:1:32:ASN:HA	1:1:36:CYS:O	0.45	2.12	18	3
1:1:51:PRO:O	1:2:59:PHE:C	0.45	2.54	33	1
1:1:45:VAL:HG23	1:1:46:PRO:N	0.45	2.27	37	3
1:1:42:ILE:CG2	1:1:45:VAL:HG13	0.45	2.42	39	7
1:1:10:GLN:CG	1:1:11:CYS:N	0.45	2.80	38	3
1:1:15:ALA:HB1	1:1:45:VAL:CG1	0.45	2.35	26	1
1:1:18:ARG:CZ	1:1:49:PHE:CE1	0.45	3.00	13	4
1:1:35:GLY:O	1:1:53:GLN:HG3	0.45	2.12	11	22
1:2:21:CYS:HB2	1:2:48:CYS:O	0.45	2.12	23	3
1:1:11:CYS:HB3	1:1:52:LEU:CD2	0.45	2.42	33	4
1:1:45:VAL:HG23	1:1:46:PRO:CD	0.45	2.42	37	2
1:2:27:THR:HG21	1:2:30:GLU:OE1	0.45	2.11	26	1
1:2:54:GLU:HB2	1:2:58:THR:HG21	0.45	1.88	37	1
1:1:10:GLN:O	1:1:13:VAL:HG12	0.45	2.11	46	1
1:1:7:SER:OG	1:1:8:ALA:N	0.45	2.50	1	2
1:1:10:GLN:C	1:1:12:ALA:N	0.45	2.70	46	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:2:8:ALA:HA	1:2:52:LEU:CD2	0.45	2.39	34	9
1:1:10:GLN:OE1	1:2:59:PHE:C	0.45	2.55	44	1
1:1:34:ARG:HG3	1:1:35:GLY:N	0.44	2.27	34	6
1:1:17:ASP:O	1:1:18:ARG:O	0.44	2.35	10	6
1:2:55:ALA:HB1	1:2:56:GLU:OE1	0.44	2.13	24	1
1:2:39:ASP:HB3	1:2:47:TRP:HA	0.44	1.89	16	4
1:2:9:ASN:N	1:2:52:LEU:HD22	0.44	2.26	18	1
1:2:11:CYS:HB3	1:2:52:LEU:CD2	0.44	2.42	21	2
1:2:26:VAL:HG22	1:2:38:PHE:CE1	0.44	2.46	29	1
1:2:37:CYS:O	1:2:49:PHE:CE1	0.44	2.70	32	1
1:2:13:VAL:CG1	1:2:17:ASP:HB3	0.44	2.43	20	7
1:1:10:GLN:NE2	1:1:51:PRO:CA	0.44	2.79	15	2
1:1:58:THR:O	1:2:51:PRO:O	0.44	2.33	16	4
1:1:57:CYS:O	1:2:53:GLN:CD	0.44	2.56	17	1
1:1:53:GLN:O	1:1:54:GLU:C	0.44	2.55	10	3
1:2:28:PRO:N	1:2:38:PHE:CE1	0.44	2.85	23	1
1:2:10:GLN:O	1:2:13:VAL:HG13	0.44	2.13	43	3
1:2:16:LYS:CE	1:2:16:LYS:O	0.44	2.66	11	2
1:2:11:CYS:HA	1:2:51:PRO:CG	0.44	2.43	29	3
1:2:53:GLN:O	1:2:57:CYS:CB	0.44	2.66	30	3
1:2:15:ALA:O	1:2:16:LYS:CG	0.44	2.66	47	12
1:1:7:SER:O	1:1:10:GLN:HB2	0.44	2.13	28	2
1:1:34:ARG:O	1:2:34:ARG:O	0.44	2.35	32	7
1:1:8:ALA:O	1:1:9:ASN:C	0.44	2.55	26	3
1:1:50:LYS:NZ	1:2:34:ARG:O	0.44	2.49	44	1
1:2:15:ALA:HB1	1:2:42:ILE:CD1	0.44	2.43	14	1
1:2:27:THR:CA	1:2:38:PHE:CE2	0.44	3.01	17	1
1:2:10:GLN:C	1:2:51:PRO:HB2	0.44	2.33	39	1
1:1:27:THR:CA	1:1:38:PHE:CE1	0.44	3.01	45	2
1:2:42:ILE:HB	1:2:45:VAL:HG13	0.44	1.89	45	2
1:1:45:VAL:CG1	1:1:46:PRO:HD2	0.44	2.43	31	2
1:2:13:VAL:HG13	1:2:14:PRO:CD	0.44	2.38	33	1
1:2:12:ALA:O	1:2:13:VAL:C	0.43	2.57	4	5
1:2:20:ASP:CG	1:2:20:ASP:O	0.43	2.55	37	10
1:1:23:TYR:CG	1:1:34:ARG:CZ	0.43	3.01	30	1
1:1:50:LYS:O	1:2:59:PHE:O	0.43	2.37	22	3
1:2:54:GLU:HA	1:2:58:THR:CG2	0.43	2.42	4	2
1:2:39:ASP:OD2	1:2:41:ARG:N	0.43	2.51	45	1
1:2:53:GLN:O	1:2:57:CYS:HB2	0.43	2.14	21	5
1:2:8:ALA:H	1:2:52:LEU:HD13	0.43	1.73	21	1
1:2:25:HIS:CD2	1:2:30:GLU:HG2	0.43	2.48	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:2:57:CYS:O	1:2:59:PHE:N	0.43	2.51	25	1
1:2:10:GLN:CG	1:2:11:CYS:N	0.43	2.82	42	1
1:2:13:VAL:CG2	1:2:14:PRO:CD	0.43	2.95	13	9
1:1:37:CYS:CB	1:1:51:PRO:HG2	0.43	2.43	36	12
1:1:16:LYS:CE	1:1:16:LYS:O	0.43	2.67	20	1
1:2:34:ARG:HG3	1:2:35:GLY:N	0.43	2.29	21	5
1:2:21:CYS:O	1:2:22:GLY:C	0.43	2.57	28	2
1:2:18:ARG:NE	1:2:49:PHE:CE2	0.43	2.86	34	1
1:1:34:ARG:NH1	1:2:34:ARG:C	0.43	2.72	24	2
1:2:39:ASP:CB	1:2:47:TRP:HA	0.43	2.43	16	5
1:2:23:TYR:CE2	1:2:34:ARG:HD3	0.43	2.48	8	1
1:1:7:SER:O	1:1:10:GLN:CB	0.43	2.66	12	1
1:2:9:ASN:H	1:2:52:LEU:HD22	0.43	1.73	18	1
1:2:11:CYS:SG	1:2:52:LEU:CD2	0.43	3.07	34	1
1:1:8:ALA:HB2	1:1:52:LEU:HD13	0.43	1.89	44	1
1:2:36:CYS:N	1:2:53:GLN:OE1	0.43	2.52	18	5
1:1:9:ASN:H	1:1:52:LEU:HD22	0.43	1.73	9	1
1:1:23:TYR:CE1	1:1:34:ARG:NE	0.43	2.86	16	1
1:2:57:CYS:C	1:2:59:PHE:N	0.43	2.72	45	2
1:1:23:TYR:CZ	1:1:34:ARG:HD3	0.43	2.49	30	1
1:1:36:CYS:N	1:1:53:GLN:OE1	0.42	2.52	1	2
1:2:10:GLN:C	1:2:12:ALA:N	0.42	2.72	18	5
1:1:54:GLU:O	1:1:58:THR:HB	0.42	2.13	44	1
1:1:19:VAL:O	1:1:19:VAL:CG1	0.42	2.67	32	2
1:1:50:LYS:O	1:2:57:CYS:O	0.42	2.37	44	1
1:1:7:SER:C	1:1:52:LEU:CB	0.42	2.87	22	1
1:2:35:GLY:O	1:2:53:GLN:CG	0.42	2.68	28	2
1:2:23:TYR:CE2	1:2:34:ARG:HB2	0.42	2.49	35	2
1:1:10:GLN:NE2	1:2:58:THR:O	0.42	2.51	38	1
1:1:58:THR:HA	1:2:53:GLN:NE2	0.42	2.30	8	2
1:1:9:ASN:O	1:1:12:ALA:CB	0.42	2.64	46	1
1:2:10:GLN:NE2	1:2:51:PRO:CA	0.42	2.78	47	1
1:1:8:ALA:HA	1:1:52:LEU:CD2	0.42	2.43	38	4
1:2:20:ASP:O	1:2:20:ASP:CG	0.42	2.58	14	10
1:1:14:PRO:O	1:1:16:LYS:HG2	0.42	2.14	40	2
1:2:15:ALA:HB2	1:2:42:ILE:HD12	0.42	1.85	39	1
1:1:50:LYS:NZ	1:2:56:GLU:OE2	0.42	2.51	46	1
1:2:11:CYS:CB	1:2:52:LEU:HD22	0.42	2.43	1	1
1:1:20:ASP:O	1:1:20:ASP:CG	0.42	2.58	22	12
1:1:57:CYS:O	1:2:50:LYS:HB2	0.42	2.15	4	4
1:1:58:THR:HA	1:2:53:GLN:CD	0.42	2.35	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:2:52:LEU:CD2	1:2:52:LEU:O	0.42	2.68	44	1
1:1:23:TYR:CE1	1:1:34:ARG:NH2	0.42	2.88	16	1
1:2:23:TYR:CZ	1:2:34:ARG:HB3	0.42	2.50	23	2
1:1:31:CYS:C	1:1:33:ASN:N	0.42	2.73	18	4
1:1:59:PHE:O	1:2:50:LYS:O	0.42	2.38	13	1
1:1:20:ASP:CG	1:1:20:ASP:O	0.42	2.57	26	2
1:1:26:VAL:HG23	1:1:48:CYS:CB	0.42	2.43	30	1
1:2:13:VAL:HG21	1:2:18:ARG:CG	0.42	2.44	36	1
1:2:37:CYS:HB2	1:2:51:PRO:HG2	0.42	1.92	1	1
1:1:13:VAL:CG2	1:1:14:PRO:CD	0.42	2.96	47	4
1:1:59:PHE:C	1:2:50:LYS:O	0.42	2.58	12	4
1:1:58:THR:O	1:2:53:GLN:OE1	0.42	2.38	8	2
1:2:7:SER:O	1:2:52:LEU:HB3	0.42	2.14	10	3
1:1:10:GLN:O	1:1:13:VAL:HB	0.42	2.15	30	2
1:1:10:GLN:OE1	1:1:51:PRO:HA	0.41	2.15	22	3
1:1:26:VAL:HG21	1:1:47:TRP:HE3	0.41	1.74	34	1
1:1:26:VAL:CG2	1:1:48:CYS:HB2	0.41	2.45	45	2
1:2:13:VAL:C	1:2:15:ALA:H	0.41	2.19	37	34
1:1:18:ARG:NE	1:1:49:PHE:CZ	0.41	2.88	2	1
1:1:23:TYR:CZ	1:1:34:ARG:HB3	0.41	2.49	28	1
1:1:13:VAL:HG13	1:1:14:PRO:HD2	0.41	1.91	38	2
1:1:13:VAL:C	1:1:15:ALA:H	0.41	2.19	43	28
1:1:34:ARG:NH2	1:2:34:ARG:O	0.41	2.54	4	1
1:1:45:VAL:HG22	1:1:46:PRO:HD3	0.41	1.90	32	2
1:2:10:GLN:CD	1:2:51:PRO:HA	0.41	2.36	45	1
1:1:50:LYS:O	1:2:59:PHE:C	0.41	2.59	33	2
1:2:30:GLU:O	1:2:34:ARG:HG2	0.41	2.15	46	9
1:2:23:TYR:CE1	1:2:34:ARG:NE	0.41	2.89	7	1
1:2:45:VAL:CG1	1:2:46:PRO:HD2	0.41	2.44	16	1
1:2:21:CYS:N	1:2:50:LYS:HZ1	0.41	2.14	25	1
1:2:27:THR:C	1:2:38:PHE:CD1	0.41	2.94	23	1
1:2:36:CYS:SG	1:2:50:LYS:CD	0.41	3.09	30	1
1:2:20:ASP:HA	1:2:46:PRO:CB	0.41	2.46	34	3
1:2:45:VAL:HG22	1:2:46:PRO:HD3	0.41	1.91	32	2
1:1:57:CYS:O	1:2:53:GLN:OE1	0.41	2.39	17	1
1:2:10:GLN:O	1:2:13:VAL:HB	0.41	2.15	29	1
1:1:51:PRO:HD2	1:1:53:GLN:HG2	0.41	1.92	34	1
1:1:9:ASN:ND2	1:1:9:ASN:C	0.41	2.74	35	1
1:1:10:GLN:OE1	1:1:51:PRO:HB3	0.41	2.16	4	2
1:1:39:ASP:OD2	1:1:41:ARG:N	0.41	2.53	29	2
1:2:35:GLY:CA	1:2:57:CYS:SG	0.41	3.09	31	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:1:11:CYS:N	1:1:51:PRO:HB2	0.41	2.31	28	2
1:1:10:GLN:O	1:1:13:VAL:HG22	0.41	2.15	6	2
1:2:36:CYS:HB3	1:2:49:PHE:O	0.41	2.15	8	1
1:1:34:ARG:NH1	1:2:34:ARG:HA	0.41	2.31	10	1
1:2:29:LYS:O	1:2:33:ASN:HB2	0.41	2.16	16	2
1:2:50:LYS:HA	1:2:53:GLN:HG2	0.41	1.92	46	2
1:2:21:CYS:SG	1:2:50:LYS:HE2	0.41	2.56	30	1
1:2:18:ARG:CZ	1:2:49:PHE:CE1	0.41	3.03	34	1
1:1:10:GLN:CG	1:1:51:PRO:HB2	0.41	2.45	40	1
1:1:31:CYS:C	1:1:36:CYS:O	0.41	2.60	41	1
1:1:13:VAL:HG12	1:1:18:ARG:HE	0.41	1.76	44	1
1:1:28:PRO:CA	1:1:38:PHE:CD1	0.41	3.04	44	1
1:1:57:CYS:C	1:1:59:PHE:N	0.41	2.72	45	1
1:2:26:VAL:HG23	1:2:31:CYS:SG	0.41	2.56	8	1
1:1:54:GLU:HB2	1:1:58:THR:CG2	0.41	2.45	15	1
1:1:20:ASP:HA	1:1:46:PRO:CB	0.41	2.46	19	1
1:2:31:CYS:C	1:2:33:ASN:N	0.41	2.75	21	2
1:1:37:CYS:CB	1:1:51:PRO:CD	0.41	2.99	45	1
1:1:27:THR:CG2	1:1:30:GLU:OE1	0.40	2.68	2	1
1:1:23:TYR:CG	1:1:34:ARG:NH2	0.40	2.88	45	1
1:1:13:VAL:CG2	1:1:17:ASP:HB3	0.40	2.47	39	1
1:2:7:SER:O	1:2:52:LEU:HB2	0.40	2.17	39	1
1:2:54:GLU:HB2	1:2:58:THR:CG2	0.40	2.46	40	1
1:2:12:ALA:C	1:2:13:VAL:O	0.40	2.60	18	1
1:1:36:CYS:HB3	1:1:49:PHE:O	0.40	2.17	35	1
1:1:54:GLU:O	1:1:54:GLU:OE2	0.40	2.39	37	1
1:1:58:THR:O	1:2:50:LYS:O	0.40	2.39	11	1
1:2:45:VAL:HG23	1:2:46:PRO:N	0.40	2.32	19	1
1:2:37:CYS:HB2	1:2:51:PRO:HD2	0.40	1.94	35	1
1:1:10:GLN:HG2	1:1:52:LEU:N	0.40	2.32	40	1
1:1:13:VAL:HG22	1:1:15:ALA:H	0.40	1.76	46	1
1:1:12:ALA:C	1:1:13:VAL:O	0.40	2.59	23	1
1:1:9:ASN:O	1:1:12:ALA:N	0.40	2.51	36	1

6.3 Torsion angles [\(i\)](#)

6.3.1 Protein backbone [\(i\)](#)

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

was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	52/59 (88%)	33±2 (64±3%)	12±2 (22±4%)	7±1 (14±3%)	1	5
1	2	52/59 (88%)	31±2 (60±3%)	13±2 (26±3%)	7±1 (14±3%)	0	5
All	All	4888/5546 (88%)	3026 (62%)	1168 (24%)	694 (14%)	1	5

All 33 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	1	16	LYS	47
1	1	20	ASP	47
1	1	29	LYS	47
1	1	51	PRO	47
1	2	16	LYS	47
1	2	20	ASP	47
1	2	29	LYS	47
1	2	51	PRO	47
1	2	9	ASN	34
1	2	54	GLU	33
1	1	13	VAL	31
1	2	13	VAL	28
1	1	9	ASN	26
1	1	54	GLU	26
1	2	8	ALA	25
1	1	55	ALA	15
1	1	8	ALA	15
1	1	15	ALA	13
1	1	18	ARG	10
1	2	15	ALA	8
1	1	17	ASP	8
1	2	18	ARG	8
1	2	55	ALA	7
1	2	17	ASP	6
1	1	39	ASP	6
1	2	26	VAL	6
1	2	39	ASP	5
1	2	53	GLN	3
1	1	7	SER	1
1	1	40	SER	1
1	1	58	THR	1
1	2	58	THR	1
1	1	26	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	1	46/51 (90%)	27±2 (58±4%)	19±2 (42±4%)	0 4
1	2	46/51 (90%)	26±2 (57±5%)	20±2 (43±5%)	0 3
All	All	4324/4794 (90%)	2475 (57%)	1849 (43%)	0 3

All 60 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	1	13	VAL	47
1	1	27	THR	47
1	1	34	ARG	47
1	1	47	TRP	47
1	1	49	PHE	47
1	1	50	LYS	47
1	1	52	LEU	47
1	2	27	THR	47
1	2	34	ARG	47
1	2	47	TRP	47
1	2	49	PHE	47
1	2	52	LEU	47
1	1	16	LYS	46
1	1	20	ASP	46
1	2	13	VAL	46
1	2	16	LYS	46
1	2	50	LYS	46
1	1	9	ASN	43
1	1	23	TYR	43
1	2	23	TYR	43
1	2	30	GLU	43
1	1	21	CYS	41
1	2	20	ASP	41
1	1	30	GLU	41
1	1	42	ILE	39
1	1	40	SER	38
1	1	45	VAL	38
1	1	54	GLU	37

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Mol	Chain	Res	Type	Models (Total)
1	2	45	VAL	37
1	1	29	LYS	35
1	2	25	HIS	34
1	2	42	ILE	34
1	2	40	SER	33
1	2	57	CYS	33
1	2	9	ASN	33
1	2	21	CYS	32
1	1	10	GLN	29
1	2	59	PHE	28
1	2	10	GLN	25
1	2	54	GLU	25
1	2	29	LYS	23
1	2	39	ASP	21
1	2	7	SER	21
1	1	56	GLU	18
1	1	7	SER	17
1	1	25	HIS	17
1	2	56	GLU	17
1	1	58	THR	13
1	1	39	ASP	11
1	1	59	PHE	10
1	2	26	VAL	9
1	2	37	CYS	8
1	2	41	ARG	8
1	1	57	CYS	7
1	1	26	VAL	6
1	2	53	GLN	6
1	2	58	THR	6
1	2	32	ASN	6
1	1	41	ARG	4
1	1	37	CYS	2

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 monosaccharides 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

No chemical shift data were provided