



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:46 PM BST

PDB ID : 1M4P
Title : Structure of the Tsg101 UEV domain in complex with a HIV-1 PTAP "late domain" peptide, DYANA Ensemble
Authors : Pornillos, O.; Alam, S.L.; Davis, D.R.; Sundquist, W.I.
Deposited on : 2002-07-03

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
<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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

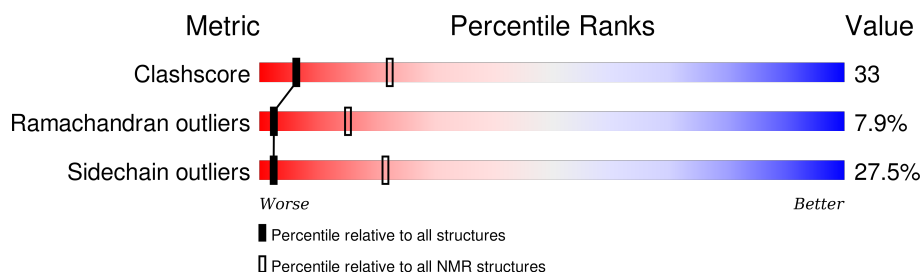
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 85%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	145	
2	B	9	

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest target function*.

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:4-A:79, A:83-A:145, B:205-B:213 (148)	0.61	5

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 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 7, 9, 10, 13, 14, 18
2	5, 6, 12, 17, 20
3	8, 15, 19
4	4, 11
Single-model clusters	3; 16

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2467 atoms, of which 1239 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tumor Susceptibility gene 101 protein.

Mol	Chain	Residues	Atoms						Trace
1	A	144	Total	C	H	N	O	S	0
			2339	757	1178	188	210	6	

- Molecule 2 is a protein called Gag Polyprotein.

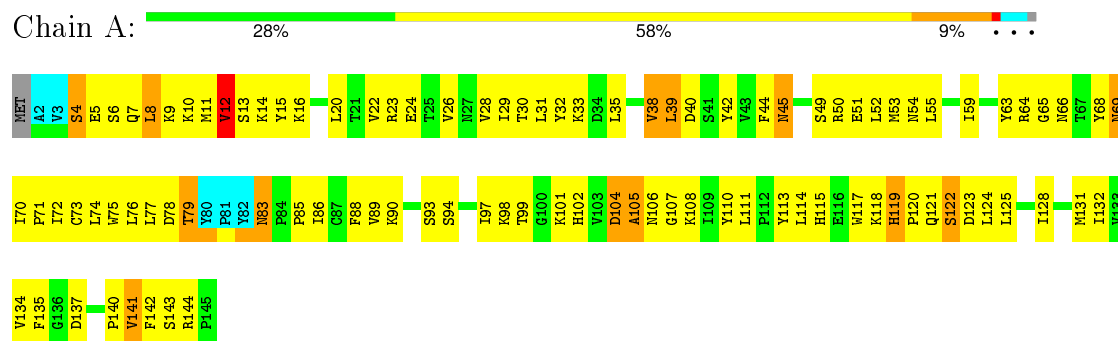
Mol	Chain	Residues	Atoms					Trace
2	B	9	Total	C	H	N	O	0
			128	42	61	9	16	

4 Residue-property plots [i](#)

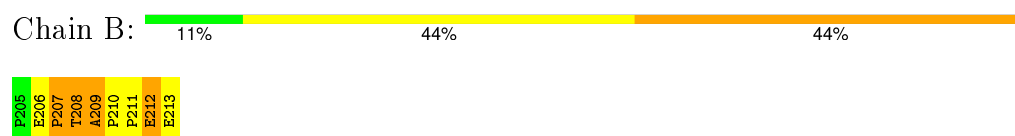
4.1 Average score per residue in the NMR ensemble

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: Tumor Susceptibility gene 101 protein



- Molecule 2: Gag Polyprotein

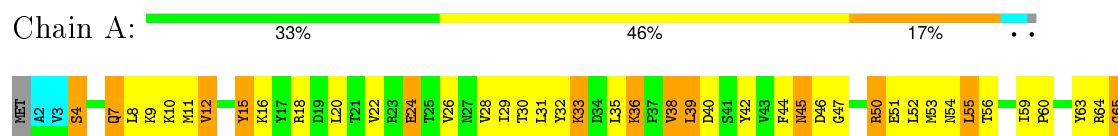


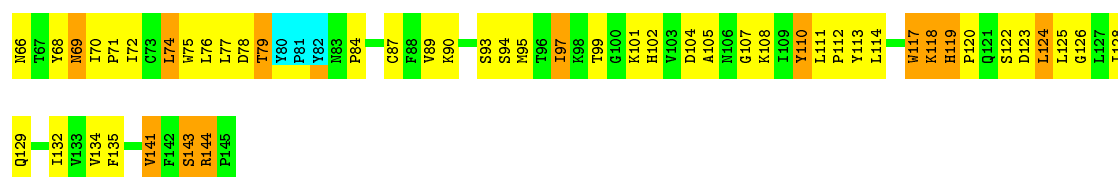
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Tumor Susceptibility gene 101 protein



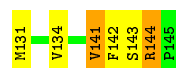
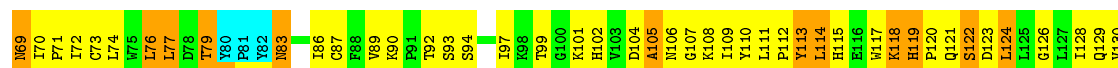
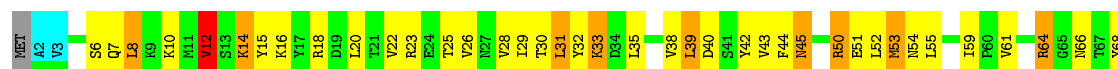


• Molecule 2: Gag Polyprotein



4.2.2 Score per residue for model 2

• Molecule 1: Tumor Susceptibility gene 101 protein

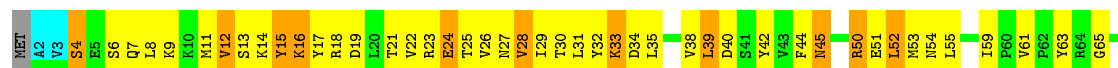


• Molecule 2: Gag Polyprotein



4.2.3 Score per residue for model 3

• Molecule 1: Tumor Susceptibility gene 101 protein



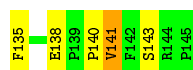


- Molecule 2: Gag Polyprotein



4.2.4 Score per residue for model 4

- Molecule 1: Tumor Susceptibility gene 101 protein

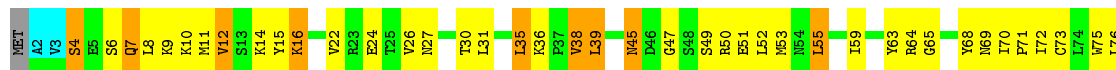


- Molecule 2: Gag Polyprotein

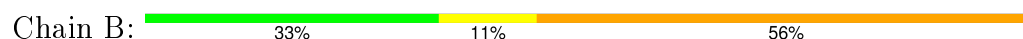


4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Tumor Susceptibility gene 101 protein



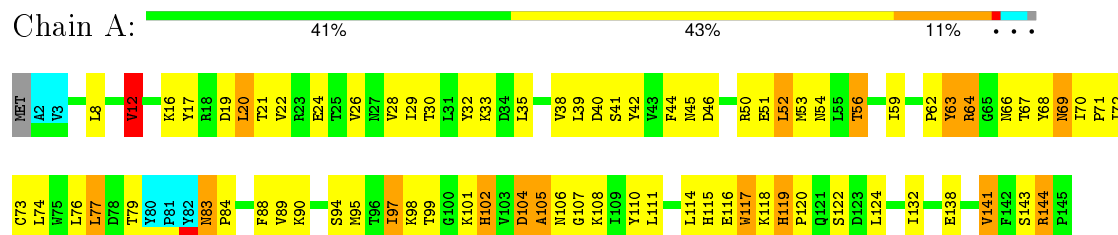
- Molecule 2: Gag Polyprotein



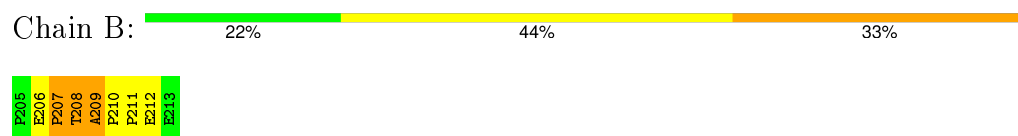


4.2.6 Score per residue for model 6

- Molecule 1: Tumor Susceptibility gene 101 protein

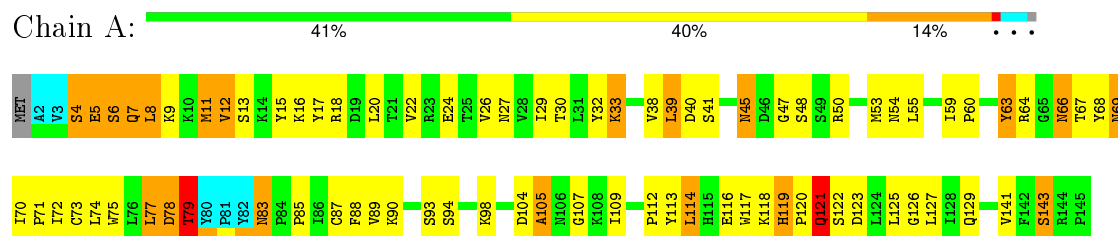


- Molecule 2: Gag Polyprotein

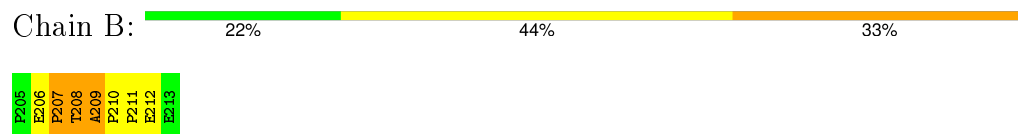


4.2.7 Score per residue for model 7

- Molecule 1: Tumor Susceptibility gene 101 protein



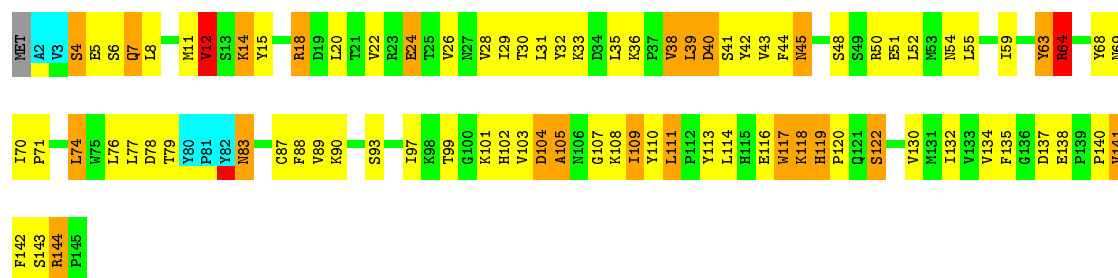
- Molecule 2: Gag Polyprotein



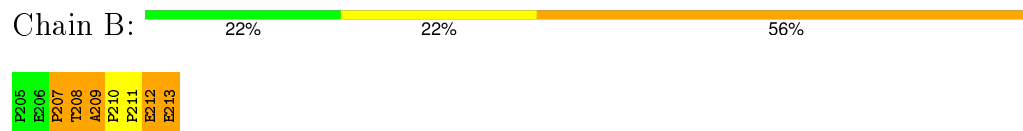
4.2.8 Score per residue for model 8

- Molecule 1: Tumor Susceptibility gene 101 protein



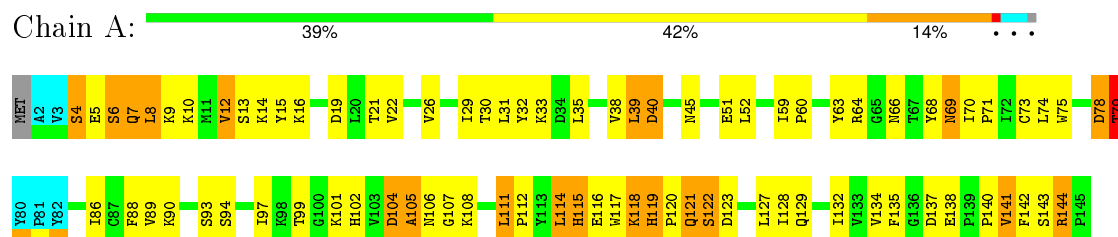


• Molecule 2: Gag Polyprotein



4.2.9 Score per residue for model 9

• Molecule 1: Tumor Susceptibility gene 101 protein

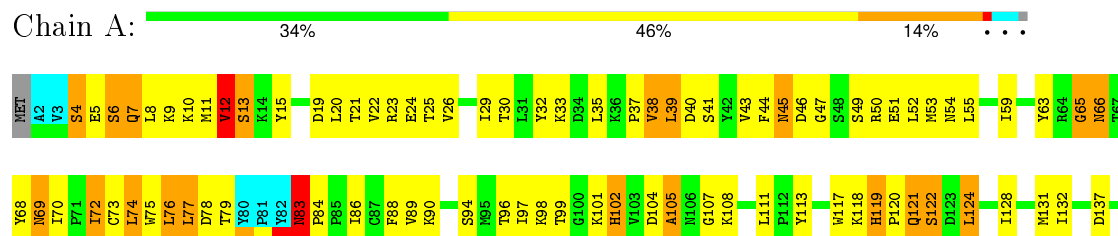


• Molecule 2: Gag Polyprotein



4.2.10 Score per residue for model 10

• Molecule 1: Tumor Susceptibility gene 101 protein





• Molecule 2: Gag Polyprotein

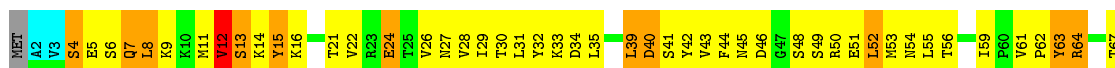
Chain B: 11% 44% 44%



4.2.11 Score per residue for model 11

• Molecule 1: Tumor Susceptibility gene 101 protein

Chain A: 24% 54% 16% . . .



• Molecule 2: Gag Polyprotein

Chain B: 33% 44% 22%



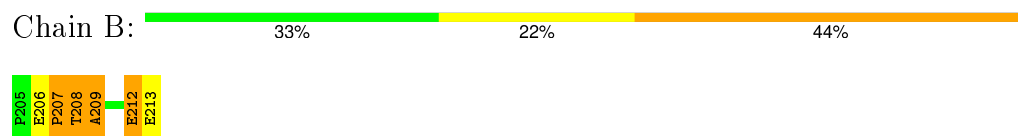
4.2.12 Score per residue for model 12

• Molecule 1: Tumor Susceptibility gene 101 protein

Chain A: 34% 43% 17% . . .

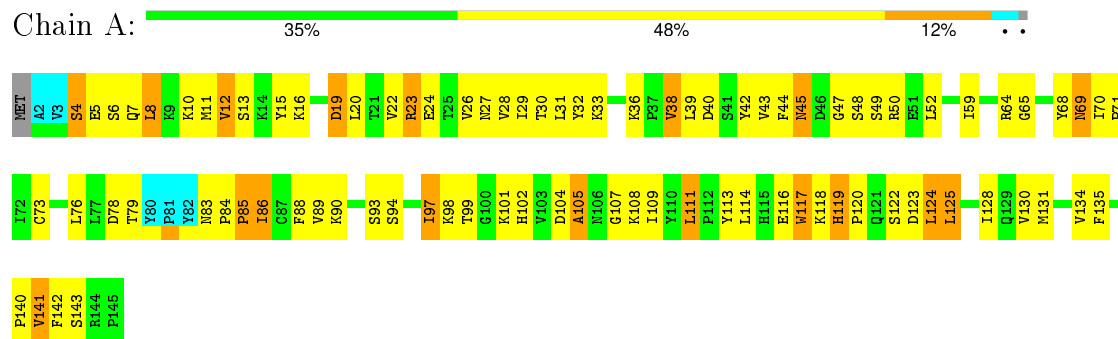


• Molecule 2: Gag Polyprotein

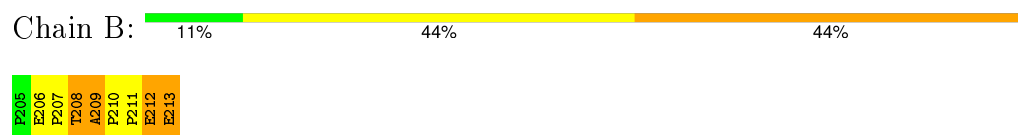


4.2.13 Score per residue for model 13

- Molecule 1: Tumor Susceptibility gene 101 protein

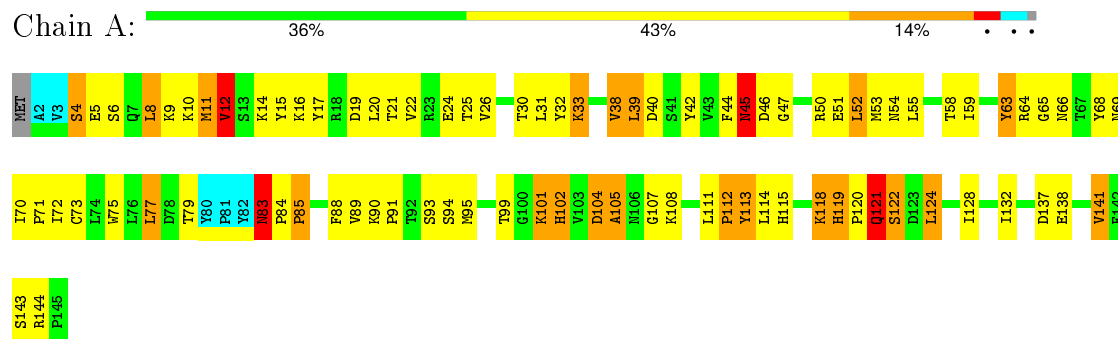


- Molecule 2: Gag Polyprotein

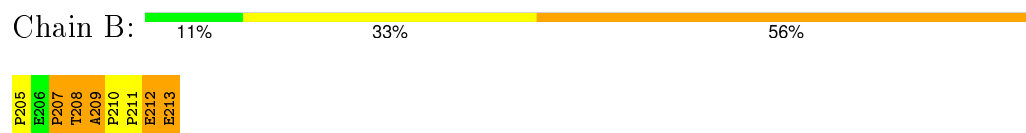


4.2.14 Score per residue for model 14

- Molecule 1: Tumor Susceptibility gene 101 protein

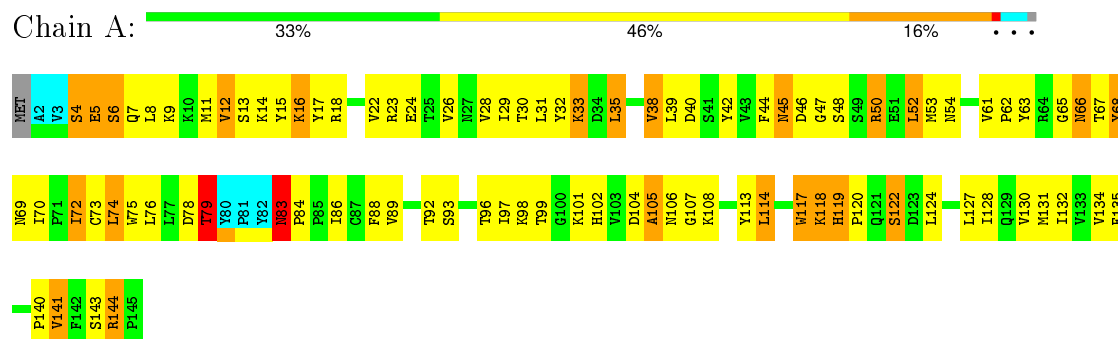


- Molecule 2: Gag Polyprotein



4.2.15 Score per residue for model 15

- Molecule 1: Tumor Susceptibility gene 101 protein

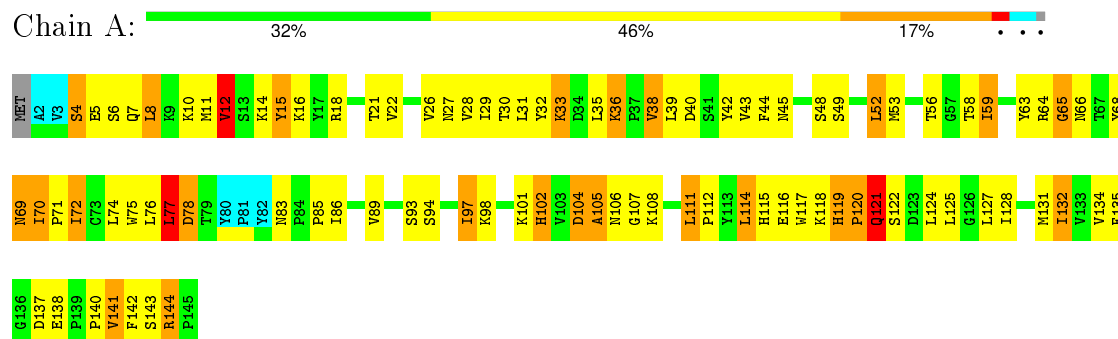


- Molecule 2: Gag Polyprotein

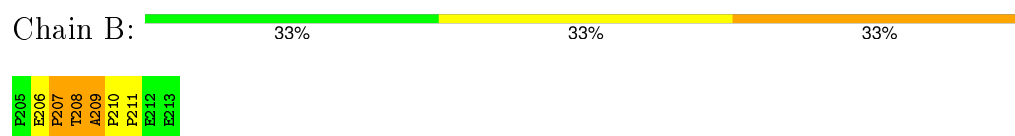


4.2.16 Score per residue for model 16

- Molecule 1: Tumor Susceptibility gene 101 protein

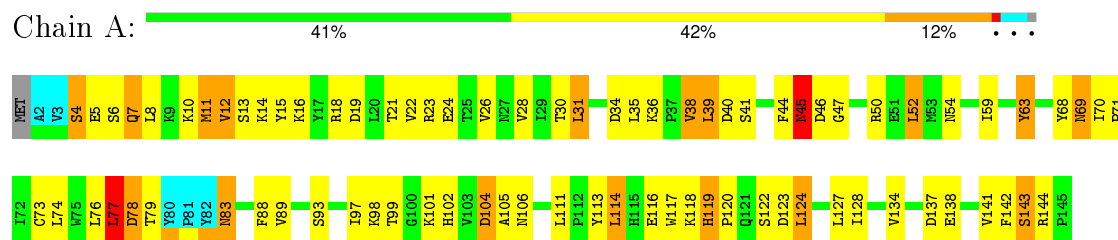


- Molecule 2: Gag Polyprotein

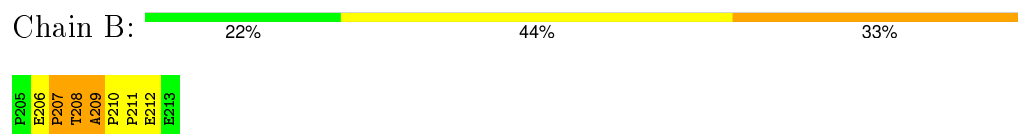


4.2.17 Score per residue for model 17

- Molecule 1: Tumor Susceptibility gene 101 protein

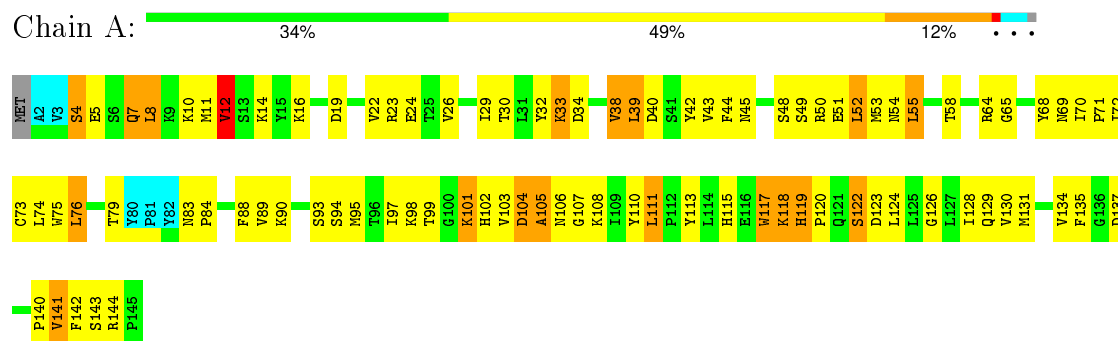


- Molecule 2: Gag Polyprotein

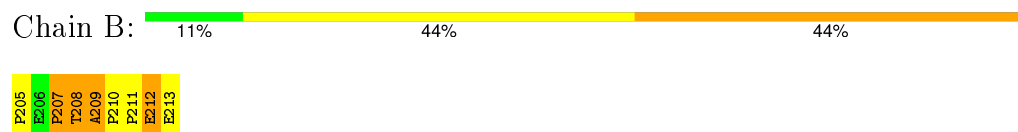


4.2.18 Score per residue for model 18

- Molecule 1: Tumor Susceptibility gene 101 protein

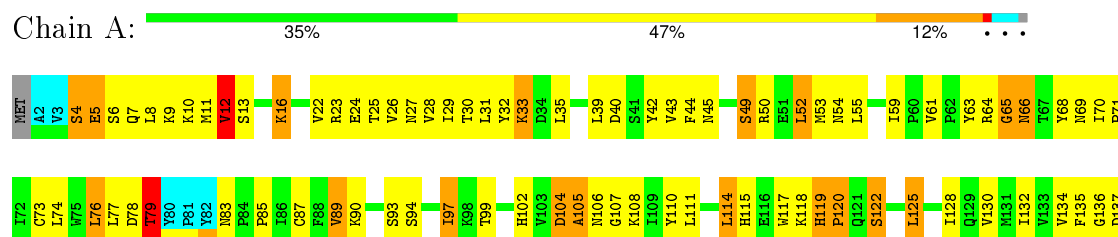


- Molecule 2: Gag Polyprotein



4.2.19 Score per residue for model 19

- Molecule 1: Tumor Susceptibility gene 101 protein



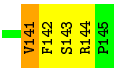


• Molecule 2: Gag Polyprotein

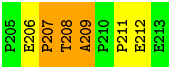
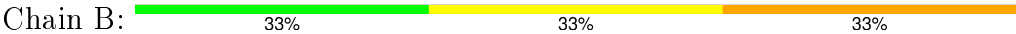


4.2.20 Score per residue for model 20

• Molecule 1: Tumor Susceptibility gene 101 protein



• Molecule 2: Gag Polyprotein



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
DYANA	structure solution	1.2
DYANA	refinement	1.2

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

Chemical shift file(s)	BMRB entry 5532
Number of chemical shift lists	2
Total number of shifts	1852
Number of shifts mapped to atoms	1852
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

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

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	1118	1139	1142	73±12
2	B	67	61	58	10±2
All	All	23700	24000	24000	1578

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 33.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:ILE:HD13	1:A:132:ILE:HD11	0.99	1.31	6	3
1:A:52:LEU:HD13	1:A:52:LEU:O	0.95	1.61	19	2
1:A:119:HIS:N	1:A:120:PRO:HA	0.94	1.77	19	20
1:A:15:TYR:CD2	1:A:21:THR:HG21	0.91	2.01	9	6
1:A:24:GLU:O	1:A:28:VAL:HG23	0.90	1.66	15	5
1:A:22:VAL:O	1:A:26:VAL:HG13	0.88	1.68	19	10
1:A:87:CYS:SG	1:A:127:LEU:HD21	0.88	2.09	11	1
1:A:71:PRO:O	1:A:89:VAL:HG23	0.87	1.69	17	12
1:A:89:VAL:HG12	1:A:107:GLY:O	0.87	1.69	4	16
1:A:76:LEU:HD11	1:A:124:LEU:HD11	0.85	1.44	5	4
1:A:8:LEU:HD13	1:A:9:LYS:N	0.84	1.87	20	1
1:A:22:VAL:O	1:A:26:VAL:HG22	0.84	1.71	10	15
1:A:76:LEU:HD11	1:A:124:LEU:HD21	0.82	1.51	18	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:LEU:HD12	1:A:8:LEU:O	0.81	1.76	18	2
1:A:52:LEU:HD21	1:A:77:LEU:HD22	0.80	1.53	20	1
1:A:35:LEU:HD13	1:A:59:ILE:HG23	0.78	1.56	3	2
1:A:101:LYS:O	1:A:111:LEU:HD11	0.78	1.79	17	1
1:A:59:ILE:HD12	1:A:132:ILE:HG12	0.76	1.58	10	6
1:A:8:LEU:C	1:A:8:LEU:HD13	0.76	2.00	20	1
1:A:111:LEU:CD1	1:A:134:VAL:HG11	0.75	2.12	8	1
1:A:52:LEU:C	1:A:52:LEU:HD22	0.75	2.02	11	2
1:A:119:HIS:N	1:A:120:PRO:CA	0.75	2.50	12	20
1:A:37:PRO:HA	1:A:55:LEU:HD23	0.75	1.59	10	2
1:A:8:LEU:O	1:A:8:LEU:HD12	0.74	1.82	9	3
1:A:52:LEU:HD11	1:A:77:LEU:HD21	0.74	1.58	20	2
1:A:99:THR:HG22	1:A:104:ASP:O	0.74	1.83	14	9
1:A:5:GLU:OE1	1:A:22:VAL:HG13	0.74	1.83	17	1
1:A:32:TYR:CZ	1:A:128:ILE:HG21	0.74	2.18	3	2
1:A:11:MET:CG	1:A:39:LEU:HD23	0.73	2.13	18	3
1:A:39:LEU:HD13	1:A:40:ASP:N	0.73	1.98	13	12
1:A:102:HIS:CE1	1:A:134:VAL:HG11	0.73	2.16	17	1
1:A:16:LYS:HB2	1:A:79:THR:HG21	0.73	1.60	19	3
1:A:97:ILE:HD11	1:A:107:GLY:HA2	0.73	1.58	3	4
1:A:39:LEU:HD11	1:A:51:GLU:HB2	0.73	1.61	4	1
1:A:8:LEU:O	1:A:12:VAL:HG22	0.72	1.84	8	15
1:A:52:LEU:HD21	1:A:77:LEU:CD2	0.72	2.14	20	1
1:A:74:LEU:N	1:A:74:LEU:HD23	0.72	1.99	15	5
1:A:52:LEU:HD22	1:A:52:LEU:C	0.72	2.05	15	1
1:A:74:LEU:HD22	1:A:74:LEU:O	0.72	1.84	1	1
1:A:52:LEU:HD11	1:A:75:TRP:CE3	0.71	2.20	11	2
1:A:109:ILE:HD11	1:A:131:MET:SD	0.71	2.26	2	3
1:A:16:LYS:CB	1:A:79:THR:HG21	0.71	2.14	5	3
1:A:135:PHE:CD2	1:A:140:PRO:CB	0.70	2.75	4	9
1:A:11:MET:HB3	1:A:39:LEU:HD23	0.69	1.63	11	4
1:A:29:ILE:HG22	1:A:35:LEU:O	0.69	1.87	15	4
1:A:113:TYR:CE1	1:A:130:VAL:HG11	0.69	2.21	3	1
1:A:32:TYR:OH	1:A:128:ILE:HG23	0.69	1.87	2	1
1:A:111:LEU:HD11	1:A:134:VAL:HG11	0.69	1.64	8	1
1:A:28:VAL:HG21	1:A:124:LEU:HD23	0.68	1.64	6	2
1:A:52:LEU:HD11	1:A:77:LEU:CD2	0.68	2.18	20	2
2:B:208:THR:O	2:B:209:ALA:HB3	0.67	1.89	4	20
1:A:102:HIS:CD2	1:A:111:LEU:HD13	0.67	2.24	16	1
1:A:52:LEU:HD11	1:A:75:TRP:CZ3	0.67	2.24	15	2
1:A:59:ILE:HD12	1:A:132:ILE:CG1	0.67	2.20	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:LEU:HD21	1:A:76:LEU:O	0.66	1.91	10	1
1:A:38:VAL:HG13	1:A:54:ASN:OD1	0.66	1.91	15	1
1:A:86:ILE:CG2	1:A:88:PHE:CE2	0.66	2.78	12	1
1:A:18:ARG:O	1:A:22:VAL:HG23	0.66	1.89	4	5
1:A:72:ILE:HD11	1:A:131:MET:SD	0.66	2.30	16	2
1:A:50:ARG:HD2	1:A:52:LEU:HD12	0.66	1.67	3	1
1:A:89:VAL:HG13	1:A:91:PRO:HD3	0.66	1.66	12	2
1:A:74:LEU:HD11	1:A:87:CYS:SG	0.66	2.31	11	1
1:A:97:ILE:HD13	1:A:105:ALA:O	0.65	1.90	19	1
1:A:96:THR:C	1:A:141:VAL:HG23	0.65	2.12	15	5
1:A:85:PRO:HB2	1:A:114:LEU:HD22	0.65	1.68	16	1
1:A:8:LEU:HD12	1:A:8:LEU:C	0.65	2.12	4	1
1:A:113:TYR:OH	1:A:134:VAL:HG21	0.65	1.92	2	1
1:A:73:CYS:O	1:A:74:LEU:HD22	0.65	1.91	19	3
1:A:74:LEU:HD13	1:A:86:ILE:O	0.65	1.91	3	3
1:A:78:ASP:O	1:A:79:THR:HG23	0.64	1.93	3	1
1:A:75:TRP:CD1	1:A:86:ILE:HG21	0.64	2.27	10	1
1:A:39:LEU:HD13	1:A:40:ASP:H	0.64	1.52	12	4
1:A:120:PRO:O	1:A:122:SER:N	0.64	2.31	11	20
1:A:12:VAL:HG12	1:A:15:TYR:CG	0.64	2.27	5	3
1:A:77:LEU:HD12	1:A:83:ASN:C	0.64	2.13	10	1
1:A:96:THR:O	1:A:141:VAL:HG23	0.64	1.92	20	2
1:A:27:ASN:HB3	1:A:125:LEU:HD11	0.63	1.69	11	2
1:A:59:ILE:CD1	1:A:132:ILE:HD11	0.63	2.19	6	2
1:A:15:TYR:CE2	1:A:21:THR:HG21	0.63	2.29	3	3
1:A:83:ASN:OD1	1:A:127:LEU:HD12	0.63	1.93	20	2
1:A:85:PRO:O	1:A:86:ILE:HD13	0.63	1.94	12	1
1:A:83:ASN:N	1:A:84:PRO:CD	0.63	2.62	4	4
1:A:102:HIS:CD2	1:A:111:LEU:HD12	0.62	2.29	6	1
1:A:8:LEU:O	1:A:8:LEU:HD22	0.62	1.94	20	1
1:A:104:ASP:O	1:A:105:ALA:HB2	0.62	1.93	16	18
1:A:27:ASN:ND2	1:A:125:LEU:HD13	0.62	2.10	19	2
1:A:12:VAL:HG12	1:A:15:TYR:CD1	0.62	2.29	5	4
1:A:44:PHE:CE2	1:A:52:LEU:HD12	0.61	2.30	18	1
1:A:117:TRP:CZ2	1:A:119:HIS:CD2	0.61	2.89	1	3
1:A:124:LEU:O	1:A:128:ILE:HD12	0.61	1.95	18	6
1:A:83:ASN:OD1	1:A:114:LEU:HD11	0.61	1.96	17	1
1:A:28:VAL:HG13	1:A:32:TYR:CE2	0.61	2.31	3	3
1:A:101:LYS:O	1:A:102:HIS:CD2	0.60	2.54	17	6
1:A:27:ASN:OD1	1:A:125:LEU:HD21	0.60	1.96	13	1
1:A:32:TYR:OH	1:A:128:ILE:HG21	0.60	1.96	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:LEU:HD13	1:A:52:LEU:C	0.60	2.17	19	2
1:A:142:PHE:CD1	1:A:142:PHE:O	0.60	2.55	11	3
1:A:74:LEU:HD22	1:A:74:LEU:C	0.60	2.17	1	1
1:A:119:HIS:CB	1:A:120:PRO:C	0.60	2.70	17	20
1:A:52:LEU:HD23	1:A:76:LEU:O	0.60	1.96	3	2
1:A:111:LEU:HD21	1:A:113:TYR:HB2	0.60	1.74	13	2
1:A:73:CYS:SG	1:A:88:PHE:CZ	0.60	2.95	11	2
1:A:15:TYR:CE2	1:A:77:LEU:O	0.60	2.55	10	5
1:A:73:CYS:O	1:A:88:PHE:CD1	0.59	2.56	14	3
1:A:111:LEU:C	1:A:111:LEU:HD23	0.59	2.17	13	1
1:A:39:LEU:HD11	1:A:51:GLU:CG	0.59	2.28	11	1
1:A:35:LEU:CD2	1:A:59:ILE:CG2	0.59	2.80	11	2
1:A:72:ILE:HD12	1:A:131:MET:SD	0.59	2.38	5	3
1:A:77:LEU:HD23	1:A:85:PRO:HB3	0.59	1.75	14	1
1:A:97:ILE:HD11	1:A:107:GLY:CA	0.58	2.28	3	5
1:A:119:HIS:HB3	1:A:120:PRO:C	0.58	2.19	16	20
1:A:127:LEU:HD23	1:A:127:LEU:C	0.58	2.17	15	2
1:A:135:PHE:CD2	1:A:140:PRO:CG	0.58	2.87	16	1
1:A:102:HIS:CE1	1:A:111:LEU:HD12	0.58	2.34	17	1
1:A:110:TYR:C	1:A:111:LEU:HD12	0.58	2.18	4	1
1:A:99:THR:CG2	1:A:104:ASP:O	0.58	2.51	10	13
1:A:79:THR:O	1:A:79:THR:HG22	0.58	1.99	17	2
1:A:39:LEU:HD22	1:A:53:MET:HA	0.58	1.75	20	3
1:A:16:LYS:O	1:A:17:TYR:CD1	0.58	2.56	15	1
1:A:39:LEU:HD23	1:A:40:ASP:H	0.58	1.58	7	1
1:A:75:TRP:CD1	1:A:86:ILE:CG2	0.58	2.87	5	3
1:A:142:PHE:O	1:A:142:PHE:CG	0.57	2.57	20	5
1:A:130:VAL:O	1:A:134:VAL:HG23	0.57	1.99	2	6
1:A:15:TYR:CD1	1:A:78:ASP:OD1	0.57	2.58	4	2
1:A:113:TYR:CE1	1:A:114:LEU:HD12	0.57	2.35	17	1
1:A:43:VAL:HG12	1:A:49:SER:N	0.57	2.15	19	4
1:A:97:ILE:HA	1:A:141:VAL:HG23	0.57	1.75	16	4
1:A:32:TYR:CE2	1:A:128:ILE:HG21	0.57	2.34	4	1
1:A:113:TYR:CG	1:A:114:LEU:N	0.57	2.71	8	4
2:B:208:THR:O	2:B:209:ALA:CB	0.57	2.51	20	20
1:A:59:ILE:HG23	1:A:60:PRO:HD2	0.57	1.77	7	3
1:A:102:HIS:NE2	1:A:134:VAL:HG13	0.57	2.15	3	2
1:A:86:ILE:HG23	1:A:88:PHE:CZ	0.57	2.35	5	3
1:A:85:PRO:HB3	1:A:114:LEU:HD13	0.57	1.77	7	1
1:A:31:LEU:HD23	1:A:32:TYR:CZ	0.57	2.35	15	2
1:A:40:ASP:OD2	1:A:75:TRP:CH2	0.56	2.58	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:VAL:HG12	1:A:15:TYR:CE1	0.56	2.35	4	3
1:A:11:MET:CB	1:A:39:LEU:HD13	0.56	2.30	7	1
1:A:110:TYR:O	1:A:111:LEU:HD22	0.56	2.00	19	2
1:A:15:TYR:CZ	1:A:77:LEU:O	0.56	2.59	7	1
1:A:55:LEU:N	1:A:55:LEU:CD2	0.56	2.69	1	3
1:A:11:MET:HG3	1:A:39:LEU:HD23	0.56	1.78	18	3
1:A:127:LEU:HD23	1:A:128:ILE:N	0.56	2.16	4	2
1:A:40:ASP:OD2	1:A:75:TRP:CZ3	0.56	2.58	16	2
1:A:113:TYR:C	1:A:113:TYR:CD1	0.55	2.79	3	3
1:A:78:ASP:O	1:A:79:THR:CG2	0.55	2.55	3	1
1:A:58:THR:HG21	2:B:205:PRO:O	0.55	2.01	14	2
1:A:43:VAL:O	1:A:44:PHE:CD1	0.55	2.60	16	7
1:A:109:ILE:HD13	1:A:131:MET:SD	0.55	2.42	12	1
1:A:59:ILE:HD13	1:A:132:ILE:CD1	0.55	2.30	16	1
1:A:86:ILE:HG22	1:A:86:ILE:O	0.55	2.01	20	1
1:A:110:TYR:O	1:A:110:TYR:CG	0.54	2.59	11	4
1:A:32:TYR:CE1	1:A:59:ILE:HD11	0.54	2.37	6	1
1:A:25:THR:HG23	1:A:55:LEU:HD21	0.54	1.79	3	2
1:A:27:ASN:CB	1:A:125:LEU:HD11	0.54	2.31	16	2
1:A:121:GLN:C	1:A:121:GLN:CD	0.54	2.66	16	3
1:A:74:LEU:N	1:A:74:LEU:CD2	0.54	2.69	15	3
1:A:42:TYR:CD2	1:A:44:PHE:CE1	0.54	2.96	2	1
1:A:62:PRO:N	1:A:67:THR:HG23	0.54	2.17	11	3
1:A:12:VAL:HG21	1:A:22:VAL:CG2	0.54	2.31	18	1
1:A:73:CYS:SG	1:A:88:PHE:CE2	0.54	3.01	13	2
1:A:111:LEU:C	1:A:111:LEU:HD22	0.54	2.23	3	1
1:A:52:LEU:HD22	1:A:53:MET:N	0.54	2.17	15	1
1:A:15:TYR:CE1	1:A:78:ASP:OD2	0.54	2.60	17	1
1:A:115:HIS:O	1:A:115:HIS:CG	0.54	2.60	12	2
1:A:28:VAL:HG12	1:A:29:ILE:N	0.54	2.17	3	2
1:A:55:LEU:CD2	1:A:55:LEU:N	0.53	2.70	18	1
1:A:119:HIS:HB2	1:A:120:PRO:O	0.53	2.04	16	20
1:A:74:LEU:CD2	1:A:74:LEU:N	0.53	2.72	10	1
1:A:110:TYR:O	1:A:110:TYR:CD2	0.53	2.61	19	2
1:A:127:LEU:C	1:A:127:LEU:HD13	0.53	2.23	17	1
1:A:142:PHE:O	1:A:142:PHE:CD1	0.53	2.62	13	1
1:A:12:VAL:CG1	1:A:15:TYR:CD2	0.53	2.92	20	3
1:A:135:PHE:CD2	1:A:140:PRO:HG3	0.53	2.39	16	1
1:A:102:HIS:CD2	1:A:134:VAL:CG1	0.53	2.91	3	1
1:A:117:TRP:CD1	1:A:120:PRO:O	0.53	2.62	20	8
1:A:15:TYR:HE2	1:A:21:THR:HG21	0.53	1.62	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:TRP:CD1	1:A:86:ILE:HG22	0.53	2.38	5	4
1:A:127:LEU:C	1:A:127:LEU:HD23	0.53	2.25	9	2
1:A:75:TRP:O	1:A:76:LEU:HD12	0.53	2.04	3	1
2:B:208:THR:HG22	2:B:209:ALA:N	0.52	2.19	20	20
1:A:53:MET:SD	1:A:76:LEU:HD22	0.52	2.44	12	1
1:A:89:VAL:HG12	1:A:107:GLY:CA	0.52	2.33	4	4
1:A:28:VAL:CG2	1:A:124:LEU:HD23	0.52	2.35	6	2
1:A:112:PRO:O	1:A:114:LEU:N	0.52	2.42	2	4
1:A:27:ASN:HD21	1:A:125:LEU:HD13	0.52	1.65	19	2
1:A:78:ASP:O	1:A:79:THR:CB	0.52	2.57	5	2
1:A:52:LEU:C	1:A:52:LEU:CD2	0.52	2.76	11	2
1:A:31:LEU:HD23	1:A:32:TYR:CE1	0.52	2.39	1	6
1:A:85:PRO:CB	1:A:114:LEU:HD22	0.52	2.33	16	1
1:A:113:TYR:CD1	1:A:114:LEU:N	0.52	2.78	11	2
1:A:32:TYR:OH	1:A:128:ILE:HD13	0.52	2.05	3	1
1:A:71:PRO:O	1:A:72:ILE:CG1	0.52	2.58	7	1
1:A:73:CYS:HB3	1:A:88:PHE:CE2	0.52	2.40	3	2
1:A:54:ASN:C	1:A:55:LEU:HD22	0.52	2.25	19	3
1:A:78:ASP:C	1:A:79:THR:HG22	0.52	2.25	5	2
1:A:110:TYR:O	1:A:111:LEU:HD12	0.52	2.05	4	1
1:A:61:VAL:C	1:A:67:THR:HG23	0.52	2.25	15	2
1:A:26:VAL:HG23	1:A:27:ASN:N	0.51	2.20	3	3
1:A:97:ILE:N	1:A:141:VAL:HG23	0.51	2.20	4	5
1:A:111:LEU:CB	1:A:113:TYR:CE2	0.51	2.93	18	2
1:A:44:PHE:HE2	1:A:52:LEU:HD12	0.51	1.65	18	1
1:A:135:PHE:CD2	1:A:140:PRO:HB3	0.51	2.40	19	7
1:A:119:HIS:CB	1:A:120:PRO:O	0.51	2.58	16	16
1:A:73:CYS:C	1:A:74:LEU:HD22	0.51	2.26	19	1
1:A:117:TRP:CH2	1:A:119:HIS:CE1	0.51	2.99	3	3
1:A:55:LEU:HD22	1:A:55:LEU:N	0.51	2.21	18	1
1:A:83:ASN:N	1:A:84:PRO:HD2	0.51	2.21	15	3
1:A:50:ARG:CZ	1:A:77:LEU:HD21	0.51	2.35	19	1
1:A:85:PRO:O	1:A:86:ILE:C	0.51	2.49	13	1
1:A:35:LEU:HD13	1:A:59:ILE:HG22	0.51	1.83	17	2
1:A:12:VAL:O	1:A:13:SER:CB	0.51	2.59	7	2
1:A:102:HIS:CE1	1:A:111:LEU:HD11	0.51	2.40	1	1
1:A:52:LEU:CD2	1:A:76:LEU:O	0.51	2.59	6	6
1:A:74:LEU:CD1	1:A:87:CYS:SG	0.51	2.99	2	3
1:A:27:ASN:CG	1:A:28:VAL:N	0.51	2.64	13	3
1:A:111:LEU:O	1:A:111:LEU:HD23	0.51	2.06	13	1
1:A:73:CYS:HB3	1:A:88:PHE:CE1	0.51	2.41	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:LEU:HB3	1:A:113:TYR:CE2	0.51	2.40	18	2
1:A:85:PRO:CB	1:A:114:LEU:HD13	0.51	2.35	7	1
1:A:71:PRO:CG	1:A:90:LYS:O	0.51	2.59	12	1
1:A:16:LYS:CA	1:A:78:ASP:O	0.51	2.59	7	1
1:A:38:VAL:CG2	1:A:39:LEU:N	0.50	2.74	5	13
1:A:11:MET:SD	1:A:39:LEU:CB	0.50	2.99	15	2
1:A:102:HIS:HA	1:A:111:LEU:HD21	0.50	1.82	11	1
1:A:38:VAL:HG13	1:A:54:ASN:ND2	0.50	2.22	14	4
1:A:52:LEU:CD2	1:A:52:LEU:C	0.50	2.79	15	1
1:A:52:LEU:CD2	1:A:53:MET:O	0.50	2.59	15	1
1:A:59:ILE:HG21	1:A:132:ILE:HG12	0.50	1.82	14	1
1:A:32:TYR:O	1:A:33:LYS:CB	0.50	2.59	20	16
1:A:142:PHE:O	1:A:142:PHE:CD2	0.50	2.65	20	1
1:A:53:MET:SD	1:A:76:LEU:CD2	0.50	2.99	12	2
1:A:26:VAL:O	1:A:30:THR:CB	0.50	2.59	16	19
1:A:127:LEU:HD23	1:A:127:LEU:O	0.50	2.06	7	1
1:A:141:VAL:O	2:B:209:ALA:CB	0.50	2.60	20	9
1:A:76:LEU:HD12	1:A:84:PRO:HG3	0.50	1.83	18	3
1:A:5:GLU:HA	1:A:8:LEU:HD23	0.50	1.83	9	1
1:A:102:HIS:CD2	1:A:111:LEU:HD21	0.50	2.42	8	1
1:A:77:LEU:HD22	1:A:78:ASP:OD1	0.50	2.07	16	1
1:A:79:THR:OG1	1:A:79:THR:O	0.50	2.29	5	4
1:A:104:ASP:O	1:A:105:ALA:CB	0.50	2.60	14	7
1:A:90:LYS:O	1:A:90:LYS:CD	0.50	2.60	11	1
1:A:74:LEU:HD13	1:A:74:LEU:N	0.50	2.22	1	1
1:A:63:TYR:O	1:A:64:ARG:CB	0.50	2.59	12	4
1:A:75:TRP:O	1:A:84:PRO:CG	0.50	2.59	18	1
1:A:11:MET:HB3	1:A:39:LEU:HD13	0.50	1.84	7	1
1:A:21:THR:HG23	1:A:76:LEU:HD21	0.50	1.83	16	1
1:A:27:ASN:OD1	1:A:28:VAL:N	0.50	2.44	13	1
1:A:50:ARG:CD	1:A:52:LEU:HD12	0.50	2.36	3	1
1:A:35:LEU:HD13	1:A:59:ILE:CG1	0.50	2.37	1	1
1:A:142:PHE:C	1:A:142:PHE:CD1	0.50	2.86	5	1
1:A:73:CYS:HB3	1:A:88:PHE:CZ	0.50	2.42	15	3
1:A:96:THR:O	1:A:141:VAL:CG2	0.50	2.60	20	1
1:A:8:LEU:O	1:A:11:MET:N	0.49	2.45	7	6
1:A:83:ASN:ND2	1:A:127:LEU:HD12	0.49	2.22	5	1
1:A:83:ASN:OD1	1:A:127:LEU:CD1	0.49	2.60	12	2
1:A:118:LYS:CG	1:A:118:LYS:O	0.49	2.59	2	1
1:A:88:PHE:CD1	1:A:88:PHE:N	0.49	2.79	3	2
1:A:28:VAL:HG22	1:A:125:LEU:HG	0.49	1.83	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:LYS:C	1:A:120:PRO:HA	0.49	2.28	1	20
1:A:32:TYR:OH	1:A:128:ILE:CG2	0.49	2.59	3	3
1:A:12:VAL:HG23	1:A:13:SER:H	0.49	1.67	9	2
1:A:79:THR:O	1:A:79:THR:HG23	0.49	2.08	4	1
1:A:18:ARG:O	1:A:22:VAL:CG2	0.49	2.60	7	1
1:A:12:VAL:HG12	1:A:15:TYR:CD2	0.49	2.42	20	1
1:A:135:PHE:CE2	1:A:140:PRO:CB	0.49	2.96	16	1
2:B:208:THR:CG2	2:B:209:ALA:N	0.49	2.76	1	20
1:A:72:ILE:HG23	1:A:73:CYS:N	0.49	2.21	20	3
1:A:73:CYS:SG	1:A:88:PHE:CE1	0.49	3.05	11	1
1:A:14:LYS:O	1:A:14:LYS:CG	0.49	2.60	18	1
1:A:87:CYS:O	1:A:109:ILE:HG22	0.49	2.07	8	1
1:A:22:VAL:O	1:A:26:VAL:CG2	0.49	2.60	5	2
1:A:79:THR:O	1:A:79:THR:CG2	0.49	2.61	17	1
1:A:111:LEU:HB3	1:A:113:TYR:CD2	0.49	2.42	18	1
1:A:89:VAL:HG12	1:A:107:GLY:C	0.49	2.26	4	3
1:A:35:LEU:HD13	1:A:59:ILE:CG2	0.49	2.38	5	4
1:A:68:TYR:CE2	2:B:210:PRO:HA	0.49	2.43	16	6
1:A:31:LEU:HD23	1:A:32:TYR:CD1	0.49	2.42	14	1
1:A:117:TRP:CZ2	1:A:119:HIS:ND1	0.49	2.81	7	2
1:A:24:GLU:O	1:A:28:VAL:CG2	0.48	2.61	19	1
1:A:24:GLU:HB3	1:A:124:LEU:HD22	0.48	1.85	4	2
1:A:88:PHE:N	1:A:88:PHE:CD1	0.48	2.81	7	3
1:A:85:PRO:HA	1:A:114:LEU:HD11	0.48	1.84	19	1
1:A:86:ILE:HG22	1:A:88:PHE:HE1	0.48	1.68	3	1
1:A:142:PHE:CG	1:A:142:PHE:O	0.48	2.65	8	4
1:A:31:LEU:HD22	1:A:125:LEU:HG	0.48	1.86	3	1
1:A:113:TYR:CE1	1:A:130:VAL:CG1	0.48	2.96	3	1
1:A:73:CYS:O	1:A:88:PHE:CE1	0.48	2.66	6	2
1:A:52:LEU:HD22	1:A:75:TRP:HE3	0.48	1.67	3	2
1:A:85:PRO:HB3	1:A:114:LEU:HD11	0.48	1.86	3	1
1:A:117:TRP:CD1	1:A:119:HIS:HB2	0.48	2.43	11	2
2:B:212:GLU:O	2:B:213:GLU:C	0.48	2.51	3	12
1:A:68:TYR:CD1	2:B:210:PRO:HB3	0.48	2.44	18	13
1:A:59:ILE:HD12	1:A:72:ILE:HG13	0.48	1.85	14	1
1:A:141:VAL:O	1:A:141:VAL:HG13	0.48	2.08	6	1
1:A:54:ASN:CB	1:A:74:LEU:O	0.48	2.62	4	1
1:A:114:LEU:O	1:A:114:LEU:HD23	0.47	2.08	14	1
1:A:59:ILE:HG21	1:A:132:ILE:CD1	0.47	2.39	1	1
1:A:84:PRO:HD2	1:A:127:LEU:HD13	0.47	1.86	20	1
1:A:59:ILE:HG21	1:A:132:ILE:HD11	0.47	1.86	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:VAL:CG2	1:A:27:ASN:N	0.47	2.77	13	3
1:A:102:HIS:CD2	1:A:134:VAL:HG13	0.47	2.44	8	3
1:A:5:GLU:OE2	1:A:29:ILE:HD11	0.47	2.09	12	1
1:A:8:LEU:C	1:A:8:LEU:HD12	0.47	2.29	18	3
1:A:16:LYS:HB3	1:A:79:THR:HG21	0.47	1.86	3	2
1:A:109:ILE:HG13	1:A:135:PHE:CZ	0.47	2.44	8	1
1:A:102:HIS:CD2	1:A:111:LEU:CD1	0.47	2.96	16	1
1:A:39:LEU:HD11	1:A:51:GLU:CB	0.47	2.37	4	1
1:A:8:LEU:HD13	1:A:53:MET:SD	0.47	2.49	11	1
1:A:35:LEU:CD2	1:A:59:ILE:HG23	0.47	2.40	11	1
1:A:53:MET:SD	1:A:76:LEU:CB	0.47	3.03	12	1
1:A:4:SER:O	1:A:6:SER:N	0.47	2.48	20	7
1:A:38:VAL:HG13	1:A:54:ASN:CG	0.47	2.30	7	2
1:A:127:LEU:CD2	1:A:127:LEU:C	0.47	2.83	15	1
1:A:17:TYR:O	1:A:20:LEU:N	0.47	2.48	7	1
1:A:15:TYR:CD1	1:A:78:ASP:HA	0.47	2.44	8	2
1:A:53:MET:SD	1:A:76:LEU:HD23	0.47	2.50	16	1
1:A:141:VAL:HG13	1:A:141:VAL:O	0.47	2.09	12	7
1:A:68:TYR:CZ	2:B:211:PRO:HD3	0.47	2.45	6	19
1:A:135:PHE:CD1	1:A:140:PRO:HB3	0.47	2.45	12	2
1:A:68:TYR:CD2	2:B:210:PRO:HA	0.47	2.45	6	4
1:A:50:ARG:CZ	1:A:77:LEU:HD11	0.47	2.39	11	1
1:A:42:TYR:HB3	1:A:44:PHE:CZ	0.47	2.45	15	11
1:A:8:LEU:C	1:A:8:LEU:CD1	0.47	2.74	20	2
1:A:38:VAL:CG1	1:A:54:ASN:OD1	0.47	2.63	15	1
1:A:35:LEU:HD13	1:A:59:ILE:HG12	0.46	1.87	1	1
1:A:102:HIS:ND1	1:A:134:VAL:HG11	0.46	2.25	17	3
1:A:135:PHE:CD2	1:A:140:PRO:HB2	0.46	2.43	4	1
1:A:27:ASN:HB3	1:A:125:LEU:HD21	0.46	1.87	7	1
1:A:111:LEU:HD13	1:A:134:VAL:HG11	0.46	1.86	8	1
1:A:35:LEU:CD1	1:A:59:ILE:CG2	0.46	2.93	17	1
1:A:101:LYS:O	1:A:102:HIS:CG	0.46	2.67	10	3
1:A:52:LEU:HD23	1:A:53:MET:O	0.46	2.10	14	1
1:A:52:LEU:CD2	1:A:77:LEU:HD22	0.46	2.34	20	1
1:A:90:LYS:CG	1:A:90:LYS:O	0.46	2.62	8	1
1:A:26:VAL:O	1:A:30:THR:N	0.46	2.47	17	9
1:A:19:ASP:OD1	1:A:20:LEU:N	0.46	2.48	13	1
1:A:15:TYR:CE1	1:A:53:MET:HB2	0.46	2.46	7	1
1:A:54:ASN:OD1	1:A:54:ASN:N	0.46	2.49	4	7
1:A:78:ASP:O	1:A:79:THR:HB	0.46	2.11	15	5
1:A:53:MET:O	1:A:76:LEU:CB	0.46	2.64	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:PRO:O	1:A:113:TYR:C	0.46	2.53	12	1
1:A:21:THR:HG23	1:A:76:LEU:CD2	0.46	2.40	16	1
1:A:87:CYS:HB2	1:A:109:ILE:HD12	0.46	1.87	3	1
1:A:83:ASN:CB	1:A:84:PRO:HD3	0.46	2.40	14	1
1:A:96:THR:HG22	1:A:142:PHE:O	0.46	2.09	20	1
1:A:111:LEU:CB	1:A:112:PRO:CD	0.46	2.94	16	1
1:A:69:ASN:ND2	2:B:206:GLU:O	0.46	2.48	7	12
1:A:27:ASN:O	1:A:31:LEU:N	0.46	2.49	3	3
1:A:29:ILE:O	1:A:33:LYS:N	0.46	2.49	19	11
1:A:68:TYR:CE2	2:B:211:PRO:HD3	0.46	2.46	3	2
1:A:63:TYR:CB	1:A:66:ASN:OD1	0.46	2.64	15	2
1:A:75:TRP:O	1:A:84:PRO:CB	0.46	2.63	18	2
1:A:54:ASN:HB3	1:A:75:TRP:CE3	0.46	2.46	7	1
1:A:12:VAL:CG1	1:A:15:TYR:CE2	0.46	2.98	8	2
1:A:89:VAL:CG1	1:A:107:GLY:O	0.46	2.62	2	1
1:A:59:ILE:N	1:A:70:ILE:O	0.46	2.49	16	1
1:A:4:SER:C	1:A:6:SER:N	0.46	2.69	20	4
1:A:86:ILE:HG22	1:A:88:PHE:CE1	0.46	2.46	3	1
1:A:97:ILE:CA	1:A:141:VAL:HG23	0.45	2.39	16	6
1:A:102:HIS:CE1	1:A:134:VAL:HG21	0.45	2.45	9	2
1:A:87:CYS:O	1:A:109:ILE:HD12	0.45	2.10	7	1
1:A:97:ILE:CG2	1:A:98:LYS:N	0.45	2.78	20	1
1:A:125:LEU:N	1:A:125:LEU:CD2	0.45	2.80	5	1
1:A:24:GLU:O	1:A:27:ASN:ND2	0.45	2.49	13	1
1:A:68:TYR:CD2	2:B:209:ALA:C	0.45	2.90	15	1
2:B:207:PRO:O	2:B:208:THR:CB	0.45	2.63	1	16
1:A:143:SER:OG	1:A:144:ARG:N	0.45	2.49	9	14
1:A:4:SER:O	1:A:8:LEU:N	0.45	2.49	16	3
1:A:66:ASN:C	1:A:67:THR:HG1	0.45	2.14	7	1
1:A:98:LYS:CG	1:A:98:LYS:O	0.45	2.65	12	1
1:A:42:TYR:O	1:A:50:ARG:N	0.45	2.49	11	8
1:A:4:SER:O	1:A:7:GLN:N	0.45	2.49	18	12
1:A:22:VAL:O	1:A:26:VAL:CG1	0.45	2.62	5	2
1:A:121:GLN:CD	1:A:122:SER:N	0.45	2.69	4	1
1:A:54:ASN:OD1	1:A:55:LEU:N	0.45	2.49	11	2
1:A:12:VAL:O	1:A:14:LYS:N	0.45	2.50	11	3
1:A:8:LEU:CD1	1:A:53:MET:SD	0.45	3.05	5	1
1:A:63:TYR:N	1:A:66:ASN:O	0.45	2.49	14	3
1:A:44:PHE:O	1:A:46:ASP:N	0.45	2.50	15	8
1:A:91:PRO:HB3	1:A:141:VAL:HG21	0.45	1.88	14	1
1:A:56:THR:O	1:A:56:THR:CG2	0.45	2.65	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:ASN:OD1	1:A:125:LEU:CD2	0.45	2.65	13	1
1:A:102:HIS:HA	1:A:111:LEU:HD11	0.45	1.87	4	1
1:A:112:PRO:O	1:A:116:GLU:N	0.45	2.50	12	1
1:A:126:GLY:O	1:A:129:GLN:N	0.45	2.50	7	3
1:A:29:ILE:O	1:A:33:LYS:CA	0.45	2.65	15	6
1:A:95:MET:HE3	2:B:207:PRO:HB2	0.45	1.89	20	1
1:A:131:MET:SD	1:A:135:PHE:CE1	0.45	3.10	13	1
1:A:110:TYR:C	1:A:111:LEU:HD22	0.45	2.31	11	1
1:A:99:THR:HG22	1:A:105:ALA:HB2	0.45	1.89	10	1
1:A:92:THR:HG23	1:A:95:MET:SD	0.45	2.52	20	1
1:A:143:SER:CB	2:B:208:THR:O	0.45	2.65	5	17
1:A:38:VAL:HG22	1:A:39:LEU:N	0.45	2.27	4	3
1:A:71:PRO:O	1:A:89:VAL:CG2	0.44	2.63	2	2
1:A:72:ILE:CG2	1:A:73:CYS:N	0.44	2.79	3	2
1:A:71:PRO:CB	1:A:90:LYS:O	0.44	2.64	9	4
1:A:112:PRO:O	1:A:115:HIS:N	0.44	2.50	12	2
1:A:40:ASP:OD1	1:A:75:TRP:CH2	0.44	2.69	7	1
1:A:86:ILE:HG22	1:A:88:PHE:CE2	0.44	2.46	12	1
1:A:117:TRP:O	1:A:118:LYS:C	0.44	2.55	13	9
1:A:32:TYR:CZ	1:A:59:ILE:HD11	0.44	2.48	6	1
1:A:52:LEU:HD22	1:A:52:LEU:O	0.44	2.11	11	1
1:A:74:LEU:HD13	1:A:74:LEU:H	0.44	1.73	1	1
1:A:40:ASP:OD2	1:A:41:SER:N	0.44	2.50	8	1
1:A:24:GLU:O	1:A:27:ASN:OD1	0.44	2.36	3	2
1:A:52:LEU:HB3	1:A:75:TRP:CZ3	0.44	2.47	3	1
1:A:65:GLY:O	1:A:66:ASN:CB	0.44	2.64	10	1
1:A:74:LEU:HD12	1:A:85:PRO:HG2	0.44	1.89	11	1
1:A:97:ILE:CD1	1:A:105:ALA:O	0.44	2.65	15	1
1:A:31:LEU:CD2	1:A:32:TYR:CE1	0.44	3.00	14	1
1:A:12:VAL:HG12	1:A:15:TYR:CZ	0.44	2.48	20	1
1:A:127:LEU:HD23	1:A:128:ILE:HG13	0.44	1.88	16	1
1:A:9:LYS:HE3	1:A:22:VAL:HG11	0.44	1.89	5	1
1:A:7:GLN:O	1:A:11:MET:N	0.44	2.50	13	4
1:A:123:ASP:O	1:A:127:LEU:N	0.44	2.49	9	1
1:A:65:GLY:C	1:A:66:ASN:ND2	0.44	2.71	4	1
1:A:128:ILE:HG22	1:A:132:ILE:CD1	0.44	2.42	15	1
1:A:9:LYS:HG3	1:A:22:VAL:HG21	0.44	1.89	15	1
1:A:55:LEU:HB2	1:A:74:LEU:HD11	0.44	1.88	1	1
1:A:15:TYR:OH	1:A:53:MET:CG	0.44	2.66	12	1
1:A:40:ASP:OD1	1:A:41:SER:N	0.44	2.51	17	3
1:A:83:ASN:CB	1:A:84:PRO:CD	0.44	2.96	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:ASN:O	1:A:55:LEU:HD22	0.44	2.13	7	2
1:A:75:TRP:O	1:A:85:PRO:CB	0.44	2.65	11	1
1:A:54:ASN:HB3	1:A:75:TRP:CZ3	0.44	2.46	7	1
1:A:15:TYR:CE1	1:A:78:ASP:HA	0.44	2.48	8	2
1:A:58:THR:HG22	2:B:207:PRO:HB3	0.44	1.89	16	1
1:A:32:TYR:CE2	1:A:128:ILE:CG2	0.44	3.01	4	1
1:A:102:HIS:HD2	1:A:111:LEU:HD11	0.44	1.71	14	1
1:A:123:ASP:O	1:A:126:GLY:N	0.44	2.51	2	6
1:A:12:VAL:C	1:A:14:LYS:N	0.44	2.70	11	2
1:A:32:TYR:OH	1:A:132:ILE:CD1	0.44	2.66	15	2
1:A:54:ASN:N	1:A:54:ASN:OD1	0.43	2.51	1	4
1:A:23:ARG:HA	1:A:26:VAL:HG22	0.43	1.90	13	2
1:A:12:VAL:HG12	1:A:15:TYR:CE2	0.43	2.48	20	2
1:A:4:SER:O	1:A:5:GLU:C	0.43	2.55	15	6
1:A:16:LYS:N	1:A:78:ASP:O	0.43	2.52	7	1
1:A:72:ILE:HD11	1:A:135:PHE:CD2	0.43	2.48	1	1
1:A:17:TYR:O	1:A:21:THR:N	0.43	2.49	14	2
1:A:121:GLN:O	1:A:122:SER:C	0.43	2.57	4	3
1:A:45:ASN:C	1:A:47:GLY:N	0.43	2.71	14	10
1:A:42:TYR:HB3	1:A:44:PHE:CE2	0.43	2.49	3	1
1:A:36:LYS:N	1:A:56:THR:O	0.43	2.51	16	2
1:A:32:TYR:CZ	1:A:132:ILE:HD11	0.43	2.48	15	1
1:A:29:ILE:CG2	1:A:35:LEU:O	0.43	2.63	15	3
1:A:61:VAL:HG13	1:A:136:GLY:HA2	0.43	1.90	19	1
1:A:15:TYR:CD2	1:A:21:THR:CG2	0.43	2.98	14	1
1:A:35:LEU:CD1	1:A:59:ILE:HG23	0.43	2.43	5	1
1:A:74:LEU:HD23	1:A:74:LEU:N	0.43	2.29	6	2
1:A:65:GLY:O	1:A:66:ASN:ND2	0.43	2.52	10	2
1:A:74:LEU:H	1:A:74:LEU:HD23	0.43	1.74	8	2
1:A:63:TYR:CE1	2:B:210:PRO:HG2	0.43	2.49	17	1
1:A:24:GLU:HA	1:A:27:ASN:ND2	0.43	2.29	13	1
2:B:213:GLU:CD	2:B:213:GLU:C	0.43	2.78	9	1
1:A:74:LEU:CB	1:A:86:ILE:O	0.43	2.67	15	1
1:A:102:HIS:CE1	1:A:111:LEU:CD1	0.43	3.02	1	1
1:A:85:PRO:O	1:A:86:ILE:CD1	0.43	2.65	12	1
1:A:72:ILE:CD1	1:A:131:MET:SD	0.43	3.05	16	1
1:A:32:TYR:CZ	1:A:132:ILE:CD1	0.42	3.02	11	1
1:A:83:ASN:N	1:A:83:ASN:OD1	0.42	2.50	10	1
1:A:52:LEU:HD13	1:A:75:TRP:CE3	0.42	2.49	18	1
1:A:103:VAL:HG22	1:A:135:PHE:CZ	0.42	2.49	8	1
1:A:88:PHE:CD1	1:A:88:PHE:O	0.42	2.72	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:THR:O	1:A:29:ILE:HG23	0.42	2.14	19	1
1:A:21:THR:O	1:A:25:THR:N	0.42	2.49	10	1
1:A:109:ILE:CD1	1:A:131:MET:SD	0.42	3.07	12	1
1:A:135:PHE:CG	1:A:140:PRO:HG3	0.42	2.49	16	1
1:A:89:VAL:N	1:A:107:GLY:O	0.42	2.50	2	1
1:A:25:THR:HG23	1:A:55:LEU:CD2	0.42	2.44	3	1
1:A:53:MET:O	1:A:76:LEU:N	0.42	2.51	2	1
1:A:52:LEU:HD22	1:A:76:LEU:O	0.42	2.15	2	1
1:A:86:ILE:CG2	1:A:88:PHE:CZ	0.42	3.01	9	1
1:A:52:LEU:HD22	1:A:75:TRP:CE3	0.42	2.50	10	2
1:A:111:LEU:HD22	1:A:112:PRO:N	0.42	2.29	3	1
1:A:14:LYS:O	1:A:15:TYR:C	0.42	2.55	16	3
1:A:121:GLN:C	1:A:121:GLN:NE2	0.42	2.73	2	1
1:A:32:TYR:OH	1:A:128:ILE:CB	0.42	2.67	3	1
1:A:78:ASP:C	1:A:79:THR:HG23	0.42	2.34	3	1
1:A:77:LEU:HD12	1:A:84:PRO:N	0.42	2.30	10	1
1:A:127:LEU:C	1:A:127:LEU:CD2	0.42	2.88	7	1
1:A:37:PRO:HA	1:A:55:LEU:CD2	0.42	2.44	20	1
1:A:123:ASP:N	1:A:123:ASP:OD1	0.42	2.52	20	1
1:A:78:ASP:OD1	1:A:79:THR:N	0.42	2.50	3	1
1:A:141:VAL:HG22	1:A:141:VAL:O	0.42	2.14	11	1
1:A:73:CYS:O	1:A:88:PHE:O	0.42	2.37	17	6
1:A:95:MET:CE	2:B:208:THR:N	0.42	2.83	1	2
1:A:15:TYR:O	1:A:16:LYS:C	0.42	2.58	4	4
1:A:112:PRO:HA	1:A:115:HIS:CD2	0.42	2.49	16	1
1:A:48:SER:O	1:A:49:SER:C	0.42	2.58	20	3
1:A:103:VAL:HG12	1:A:104:ASP:H	0.42	1.73	11	1
1:A:16:LYS:C	1:A:17:TYR:CG	0.42	2.93	15	1
1:A:65:GLY:C	1:A:66:ASN:CG	0.42	2.78	19	2
1:A:32:TYR:CZ	1:A:59:ILE:HG21	0.42	2.50	2	1
1:A:55:LEU:N	1:A:55:LEU:HD23	0.42	2.30	1	1
1:A:74:LEU:CD1	1:A:74:LEU:N	0.42	2.83	1	1
1:A:23:ARG:O	1:A:27:ASN:OD1	0.41	2.38	19	2
1:A:89:VAL:HG22	1:A:90:LYS:N	0.41	2.30	10	1
1:A:65:GLY:O	1:A:66:ASN:CG	0.41	2.59	16	2
1:A:54:ASN:CG	1:A:55:LEU:N	0.41	2.74	19	1
1:A:11:MET:O	1:A:11:MET:CG	0.41	2.67	13	1
1:A:121:GLN:NE2	1:A:121:GLN:C	0.41	2.74	9	1
1:A:12:VAL:HG11	1:A:15:TYR:CD2	0.41	2.50	3	2
1:A:113:TYR:CD1	1:A:113:TYR:C	0.41	2.93	15	1
1:A:123:ASP:O	1:A:124:LEU:C	0.41	2.59	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:TYR:CG	1:A:110:TYR:O	0.41	2.71	5	1
1:A:7:GLN:O	1:A:11:MET:CB	0.41	2.68	13	1
1:A:111:LEU:HD21	1:A:113:TYR:CB	0.41	2.45	13	1
2:B:213:GLU:C	2:B:213:GLU:CD	0.41	2.78	13	3
1:A:79:THR:O	1:A:79:THR:OG1	0.41	2.39	1	2
1:A:87:CYS:HB3	1:A:109:ILE:HD13	0.41	1.92	4	1
1:A:102:HIS:O	1:A:110:TYR:N	0.41	2.50	1	1
1:A:43:VAL:HG12	1:A:49:SER:CA	0.41	2.45	16	1
1:A:73:CYS:CB	1:A:88:PHE:CE2	0.41	3.03	3	1
1:A:83:ASN:OD1	1:A:83:ASN:C	0.41	2.58	14	1
1:A:74:LEU:C	1:A:74:LEU:CD2	0.41	2.87	1	1
1:A:110:TYR:O	1:A:111:LEU:C	0.41	2.59	6	2
1:A:102:HIS:CD2	1:A:111:LEU:HD11	0.41	2.50	14	1
1:A:141:VAL:O	1:A:141:VAL:HG22	0.41	2.16	8	1
1:A:13:SER:C	1:A:15:TYR:N	0.41	2.73	12	1
1:A:32:TYR:CZ	1:A:59:ILE:CG2	0.41	3.04	2	1
1:A:143:SER:O	1:A:144:ARG:O	0.41	2.39	2	1
1:A:20:LEU:O	1:A:24:GLU:CB	0.41	2.69	6	1
1:A:52:LEU:HD11	1:A:75:TRP:HE3	0.41	1.67	11	1
1:A:118:LYS:O	1:A:118:LYS:CD	0.41	2.69	2	1
1:A:28:VAL:O	1:A:31:LEU:N	0.41	2.51	4	4
1:A:38:VAL:O	1:A:54:ASN:O	0.41	2.39	20	2
1:A:12:VAL:O	1:A:13:SER:C	0.41	2.59	11	1
1:A:117:TRP:CZ2	1:A:119:HIS:CE1	0.41	3.08	7	1
1:A:8:LEU:C	1:A:10:LYS:N	0.41	2.74	1	1
1:A:84:PRO:O	1:A:87:CYS:SG	0.41	2.79	1	1
1:A:85:PRO:O	1:A:86:ILE:O	0.41	2.39	20	1
1:A:117:TRP:CD1	1:A:122:SER:HB2	0.41	2.51	2	1
1:A:25:THR:CG2	1:A:55:LEU:HD21	0.41	2.46	2	1
1:A:39:LEU:C	1:A:39:LEU:HD13	0.41	2.37	13	1
1:A:52:LEU:HD22	1:A:53:MET:O	0.41	2.16	15	1
1:A:121:GLN:CD	1:A:121:GLN:C	0.41	2.80	7	1
1:A:24:GLU:OE1	1:A:125:LEU:CD1	0.41	2.69	1	1
1:A:71:PRO:HG3	2:B:207:PRO:CB	0.41	2.46	8	1
1:A:7:GLN:O	1:A:11:MET:SD	0.40	2.79	17	1
1:A:129:GLN:O	1:A:133:VAL:HG23	0.40	2.16	11	1
1:A:78:ASP:N	1:A:78:ASP:OD1	0.40	2.55	11	1
1:A:11:MET:HG3	1:A:39:LEU:CD2	0.40	2.45	18	1
1:A:64:ARG:O	1:A:64:ARG:NH1	0.40	2.54	2	1
1:A:101:LYS:O	1:A:111:LEU:CD1	0.40	2.62	17	1
1:A:44:PHE:CD2	1:A:50:ARG:CZ	0.40	3.03	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:112:PRO:C	1:A:114:LEU:N	0.40	2.75	9	1
1:A:24:GLU:C	1:A:27:ASN:OD1	0.40	2.59	3	1
1:A:19:ASP:N	1:A:19:ASP:OD1	0.40	2.54	10	1
1:A:40:ASP:OD1	1:A:52:LEU:O	0.40	2.40	18	2
1:A:98:LYS:O	1:A:103:VAL:CG2	0.40	2.69	12	1
1:A:23:ARG:O	1:A:27:ASN:CG	0.40	2.60	12	1
1:A:54:ASN:OD1	1:A:74:LEU:O	0.40	2.39	19	1
1:A:103:VAL:HG12	1:A:104:ASP:N	0.40	2.31	18	1
1:A:100:GLY:O	1:A:101:LYS:HB2	0.40	2.17	12	1
1:A:111:LEU:C	1:A:111:LEU:CD2	0.40	2.88	13	1
1:A:110:TYR:O	1:A:111:LEU:CD1	0.40	2.69	4	1
1:A:119:HIS:HB3	1:A:121:GLN:CB	0.40	2.46	11	2
1:A:40:ASP:O	1:A:40:ASP:OD1	0.40	2.39	18	1
1:A:59:ILE:CD1	1:A:132:ILE:CG1	0.40	2.99	8	1
1:A:102:HIS:CE1	1:A:111:LEU:HG	0.40	2.52	9	1
1:A:12:VAL:HG13	1:A:53:MET:CG	0.40	2.47	3	1
1:A:26:VAL:O	1:A:30:THR:OG1	0.40	2.39	10	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	138/145 (95%)	103±4 (75±3%)	25±4 (18±3%)	9±2 (7±1%)	3	18
2	B	7/9 (78%)	4±1 (50±10%)	2±1 (21±10%)	2±0 (29±0%)	0	1
All	All	2900/3080 (94%)	2138 (74%)	534 (18%)	228 (8%)	2	15

All 32 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	141	VAL	20
2	B	209	ALA	20
1	A	45	ASN	20
1	A	105	ALA	20

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Mol	Chain	Res	Type	Models (Total)
2	B	207	PRO	20
1	A	79	THR	16
1	A	117	TRP	13
1	A	12	VAL	12
1	A	65	GLY	11
1	A	102	HIS	10
1	A	83	ASN	10
1	A	122	SER	8
1	A	121	GLN	7
1	A	77	LEU	4
1	A	113	TYR	4
1	A	120	PRO	3
1	A	15	TYR	3
1	A	66	ASN	3
1	A	64	ARG	3
1	A	86	ILE	3
1	A	85	PRO	2
1	A	144	ARG	2
1	A	49	SER	2
1	A	95	MET	2
1	A	92	THR	2
1	A	5	GLU	2
1	A	100	GLY	1
1	A	13	SER	1
1	A	76	LEU	1
1	A	106	ASN	1
1	A	112	PRO	1
1	A	97	ILE	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	131/136 (96%)	95±4 (73±3%)	36±4 (27±3%)	2	22
2	B	8/8 (100%)	6±1 (71±8%)	2±1 (29±8%)	2	19
All	All	2780/2880 (97%)	2015 (72%)	765 (28%)	2	21

All 94 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	119	HIS	20
2	B	208	THR	20
1	A	70	ILE	20
1	A	69	ASN	20
1	A	12	VAL	19
2	B	212	GLU	18
1	A	4	SER	17
1	A	39	LEU	16
1	A	7	GLN	16
1	A	94	SER	15
1	A	108	LYS	15
1	A	52	LEU	15
1	A	38	VAL	15
1	A	16	LYS	15
1	A	63	TYR	15
1	A	64	ARG	14
1	A	93	SER	14
1	A	50	ARG	14
1	A	6	SER	13
1	A	24	GLU	13
1	A	83	ASN	12
1	A	137	ASP	12
1	A	8	LEU	12
1	A	51	GLU	12
1	A	104	ASP	12
1	A	114	LEU	12
1	A	10	LYS	11
1	A	106	ASN	11
1	A	124	LEU	11
1	A	101	LYS	11
1	A	77	LEU	10
1	A	115	HIS	10
1	A	98	LYS	10
1	A	78	ASP	10
1	A	97	ILE	10
1	A	118	LYS	9
1	A	5	GLU	9
1	A	33	LYS	9
1	A	144	ARG	9
1	A	116	GLU	9
1	A	138	GLU	9

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Mol	Chain	Res	Type	Models (Total)
1	A	9	LYS	8
1	A	90	LYS	8
1	A	13	SER	8
1	A	36	LYS	8
1	A	23	ARG	7
1	A	79	THR	7
1	A	111	LEU	7
1	A	74	LEU	7
1	A	19	ASP	7
1	A	76	LEU	7
1	A	20	LEU	7
1	A	53	MET	7
1	A	14	LYS	7
1	A	72	ILE	6
1	A	48	SER	6
2	B	213	GLU	6
1	A	45	ASN	6
1	A	18	ARG	5
1	A	31	LEU	5
1	A	40	ASP	5
1	A	143	SER	5
1	A	55	LEU	5
1	A	129	GLN	5
1	A	66	ASN	5
1	A	35	LEU	5
1	A	34	ASP	5
1	A	125	LEU	4
1	A	122	SER	4
1	A	49	SER	4
1	A	121	GLN	3
1	A	42	TYR	3
1	A	123	ASP	3
1	A	11	MET	3
1	A	110	TYR	3
2	B	206	GLU	2
1	A	132	ILE	2
1	A	15	TYR	2
1	A	41	SER	2
1	A	95	MET	2
1	A	59	ILE	2
1	A	131	MET	2
1	A	113	TYR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	61	VAL	2
1	A	87	CYS	2
1	A	56	THR	2
1	A	89	VAL	1
1	A	28	VAL	1
1	A	68	TYR	1
1	A	17	TYR	1
1	A	130	VAL	1
1	A	109	ILE	1
1	A	103	VAL	1
1	A	102	HIS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 85% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5532

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1760
Number of shifts mapped to atoms	1760
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	139	0.04 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	131	0.50 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	128	0.01 ± 0.17	None needed (< 0.5 ppm)
^{15}N	130	0.38 ± 0.38	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 80%, i.e. 1488 atoms were assigned a chemical shift out of a possible 1858. 28 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	648/708 (92%)	264/280 (94%)	258/296 (87%)	126/132 (95%)
Sidechain	764/1005 (76%)	466/594 (78%)	288/375 (77%)	10/36 (28%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	76/145 (52%)	41/76 (54%)	33/64 (52%)	2/5 (40%)
Overall	1488/1858 (80%)	771/950 (81%)	579/735 (79%)	138/173 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1541 atoms were assigned a chemical shift out of a possible 1920. 29 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	670/731 (92%)	273/289 (94%)	267/306 (87%)	130/136 (96%)
Sidechain	787/1028 (77%)	480/608 (79%)	297/384 (77%)	10/36 (28%)
Aromatic	84/161 (52%)	45/84 (54%)	37/72 (51%)	2/5 (40%)
Overall	1541/1920 (80%)	798/981 (81%)	601/762 (79%)	142/177 (80%)

7.1.4 Statistically unusual chemical shifts ⓘ

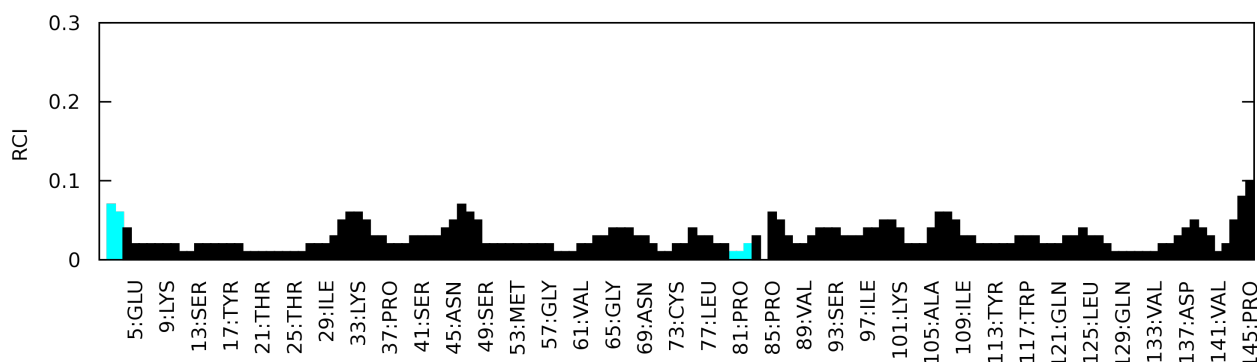
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	80	TYR	CE1	133.20	124.14 – 111.74	12.3
1	A	122	SER	HB2	1.17	5.18 – 2.58	-10.4
1	A	54	ASN	HD21	3.74	9.74 – 4.94	-7.5
1	A	81	PRO	HG2	-0.39	3.48 – 0.38	-7.5
1	A	42	TYR	HD1	4.76	8.44 – 5.44	-7.3
1	A	122	SER	HB3	1.88	5.25 – 2.45	-7.0
1	A	140	PRO	HG2	0.03	3.48 – 0.38	-6.1
1	A	81	PRO	HA	2.53	6.05 – 2.75	-5.7
1	A	78	ASP	HA	2.96	6.15 – 3.05	-5.3

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: BMRB entry 5532

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 Bookkeeping ⓘ

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

Total number of shifts	92
Number of shifts mapped to atoms	92
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.2.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	8	1.13 ± 0.20	Should be applied
$^{13}\text{C}_\beta$	9	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	5	-1.39 ± 1.88	None needed (imprecise)
^{15}N	5	-0.83 ± 4.79	None needed (imprecise)

7.2.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 5%, i.e. 85 atoms were assigned a chemical shift out of a possible 1858. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	32/708 (5%)	14/280 (5%)	13/296 (4%)	5/132 (4%)
Sidechain	53/1005 (5%)	33/594 (6%)	20/375 (5%)	0/36 (0%)
Aromatic	0/145 (0%)	0/76 (0%)	0/64 (0%)	0/5 (0%)
Overall	85/1858 (5%)	47/950 (5%)	33/735 (4%)	5/173 (3%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 85 atoms were assigned a chemical shift out of a possible 1920. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	32/731 (4%)	14/289 (5%)	13/306 (4%)	5/136 (4%)
Sidechain	53/1028 (5%)	33/608 (5%)	20/384 (5%)	0/36 (0%)
Aromatic	0/161 (0%)	0/84 (0%)	0/72 (0%)	0/5 (0%)
Overall	85/1920 (4%)	47/981 (5%)	33/762 (4%)	5/177 (3%)

7.2.4 Statistically unusual chemical shifts ⓘ

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

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	207	PRO	C	150.59	184.42 – 169.02	-17.0
2	B	205	PRO	C	156.21	184.42 – 169.02	-13.3

7.2.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain B:

