



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 11:41 PM UTC

PDB ID : 1M4Q / pdb_00001m4q
Title : STRUCTURE OF THE TSG101 UEV DOMAIN IN COMPLEX WITH A
HIV-1 PTAP "LATE DOMAIN" PEPTIDE, CNS 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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

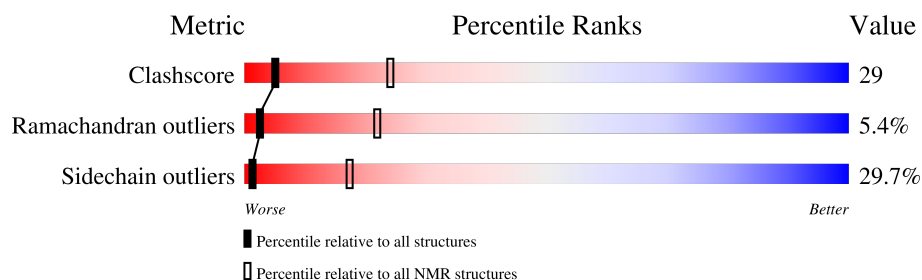
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

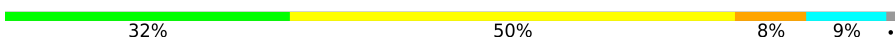
The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	145	
2	B	9	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models). The authors have identified model 8 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:42, A:50-A:78, A:83-A:145, B:205-B:213 (140)	0.86	1

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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2474 atoms, of which 1244 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
			2346	757	1184	188	211	6	

- Molecule 2 is a protein called Gag Polyprotein.

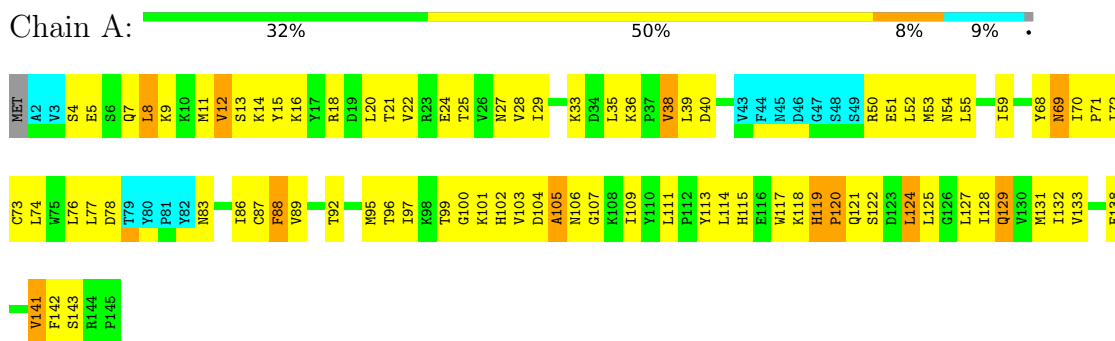
Mol	Chain	Residues	Atoms					Trace
2	B	9	Total	C	H	N	O	0
			128	42	60	9	17	

4 Residue-property plots

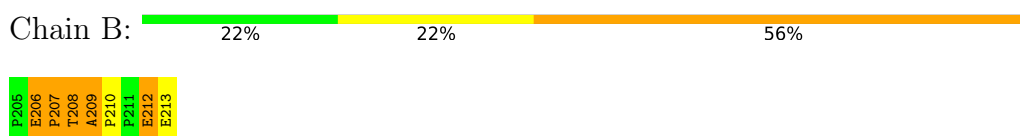
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Tumor Susceptibility gene 101 protein



- Molecule 2: Gag Polyprotein

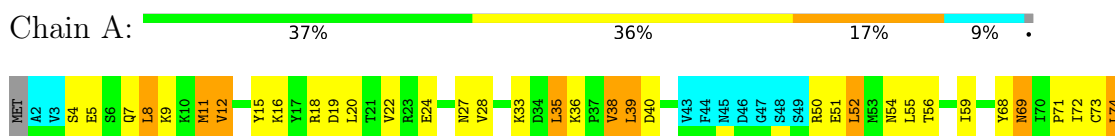


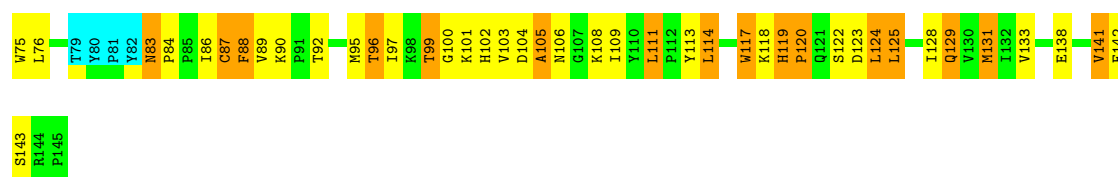
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

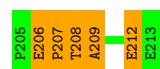
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Tumor Susceptibility gene 101 protein



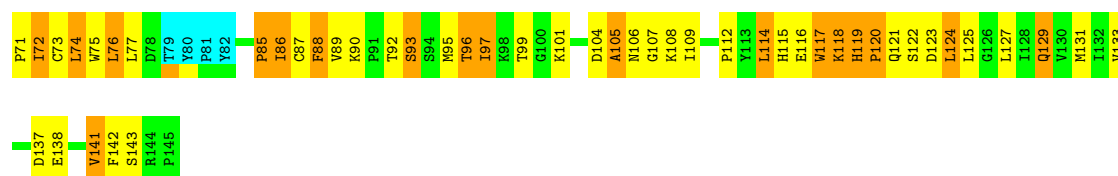
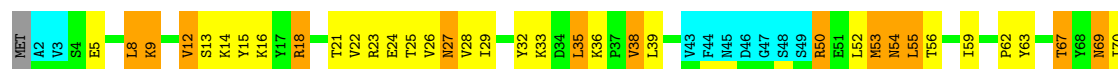


- Molecule 2: Gag Polyprotein

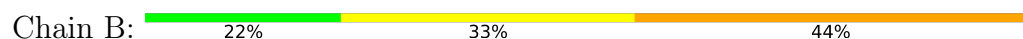


4.2.2 Score per residue for model 2

- Molecule 1: Tumor Susceptibility gene 101 protein

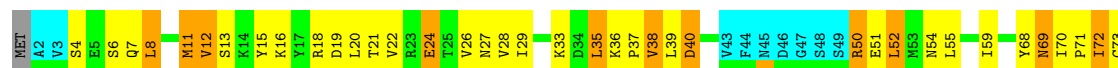


- Molecule 2: Gag Polyprotein



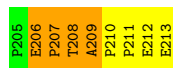
4.2.3 Score per residue for model 3

- Molecule 1: Tumor Susceptibility gene 101 protein



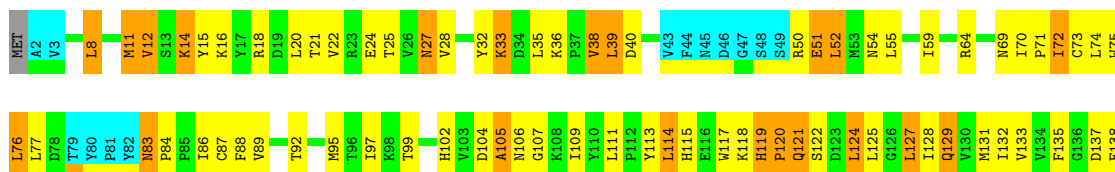


• Molecule 2: Gag Polyprotein

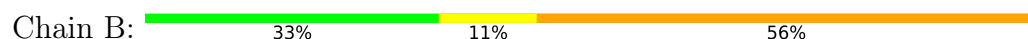


4.2.4 Score per residue for model 4

• Molecule 1: Tumor Susceptibility gene 101 protein

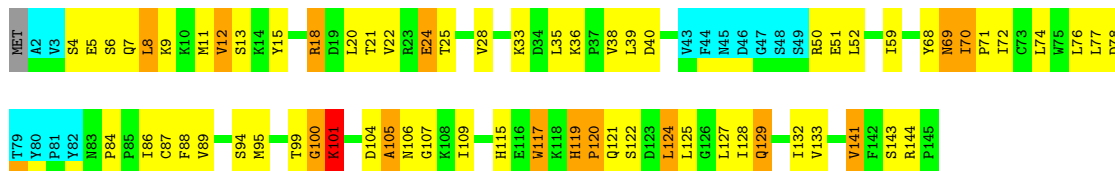


• Molecule 2: Gag Polyprotein

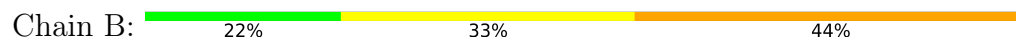


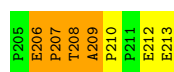
4.2.5 Score per residue for model 5

• Molecule 1: Tumor Susceptibility gene 101 protein



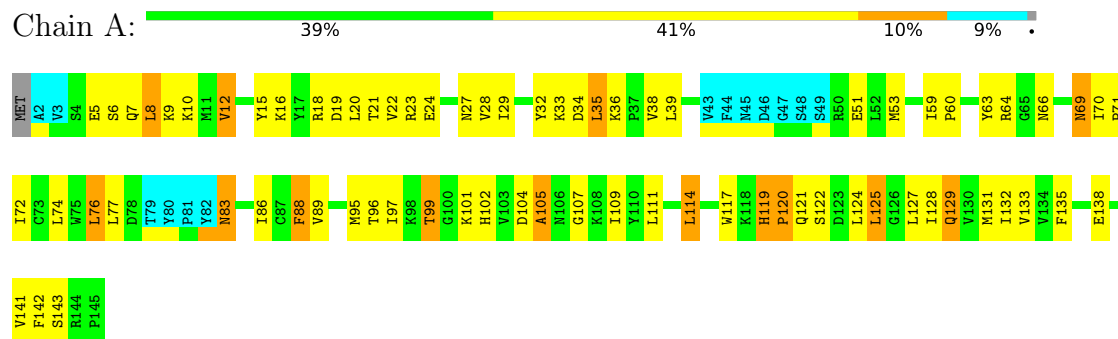
• Molecule 2: Gag Polyprotein



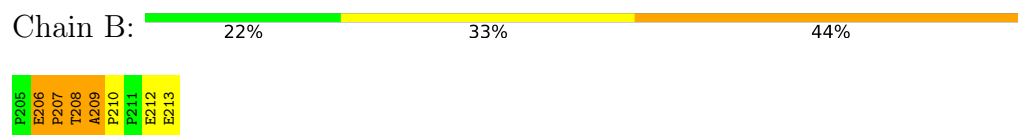


4.2.6 Score per residue for model 6

- Molecule 1: Tumor Susceptibility gene 101 protein

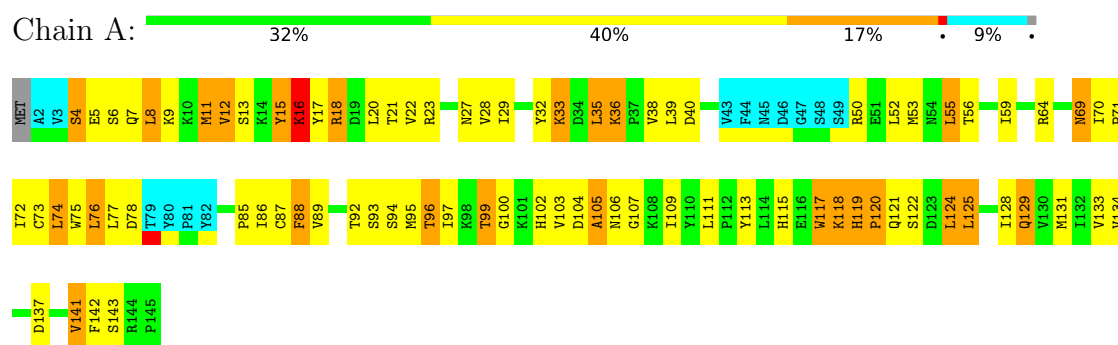


- Molecule 2: Gag Polyprotein

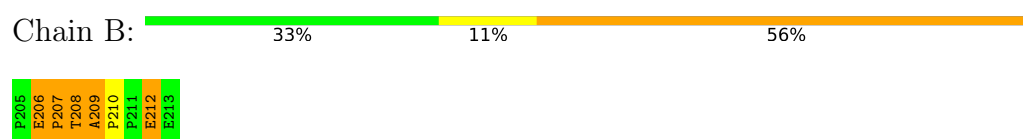


4.2.7 Score per residue for model 7

- Molecule 1: Tumor Susceptibility gene 101 protein

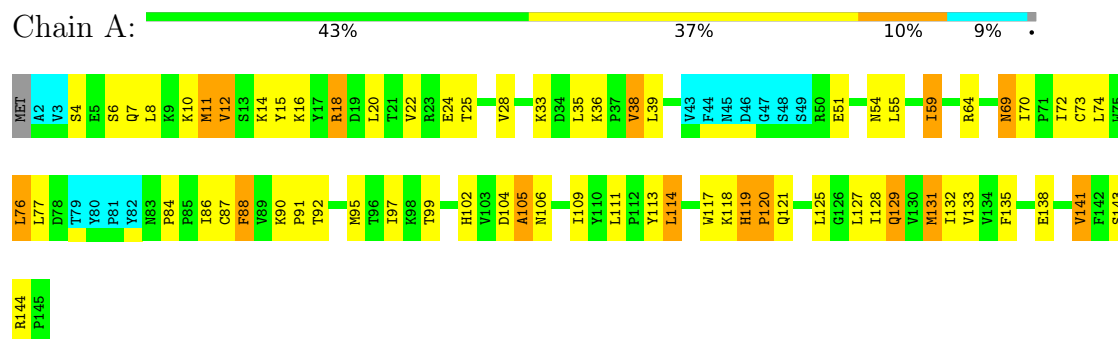


- Molecule 2: Gag Polyprotein

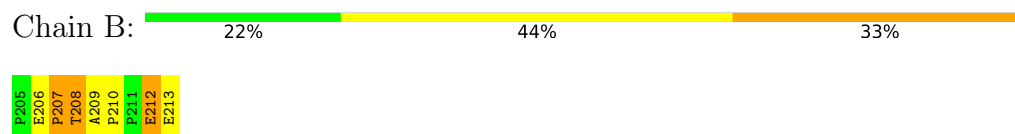


4.2.8 Score per residue for model 8

- Molecule 1: Tumor Susceptibility gene 101 protein

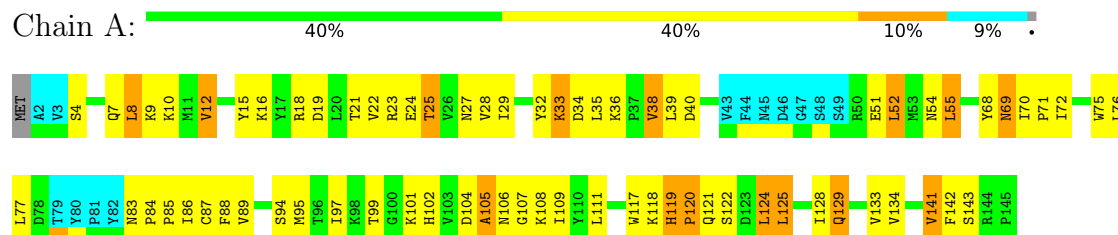


- Molecule 2: Gag Polyprotein

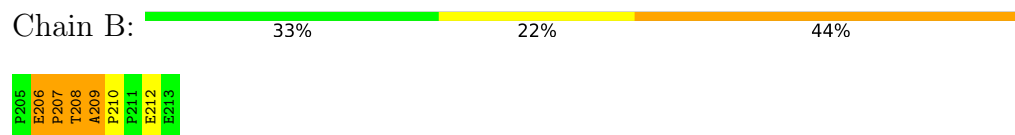


4.2.9 Score per residue for model 9

- Molecule 1: Tumor Susceptibility gene 101 protein



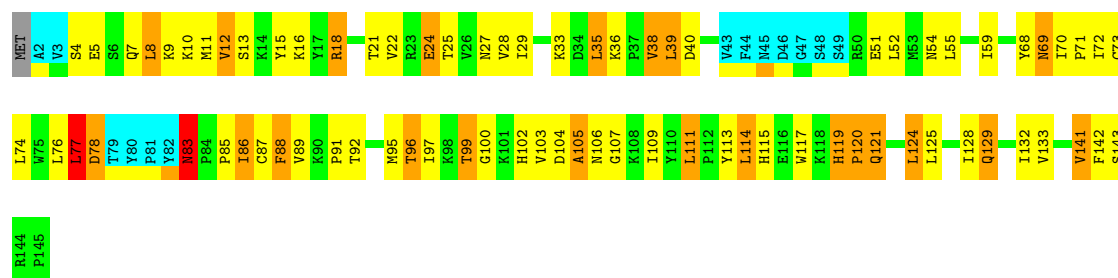
- Molecule 2: Gag Polyprotein



4.2.10 Score per residue for model 10

- Molecule 1: Tumor Susceptibility gene 101 protein





• Molecule 2: Gag Polyprotein

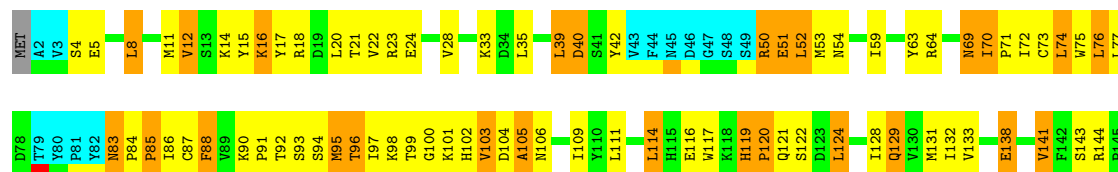
Chain B: 22% 22% 56%



4.2.11 Score per residue for model 11

• Molecule 1: Tumor Susceptibility gene 101 protein

Chain A: 35% 37% 18% 9%



• Molecule 2: Gag Polyprotein

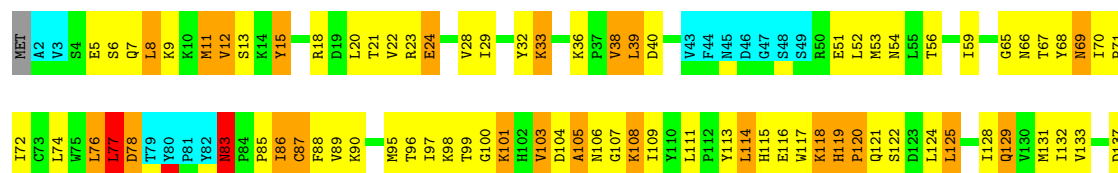
Chain B: 33% 22% 44%



4.2.12 Score per residue for model 12

• Molecule 1: Tumor Susceptibility gene 101 protein

Chain A: 32% 40% 17% 9%



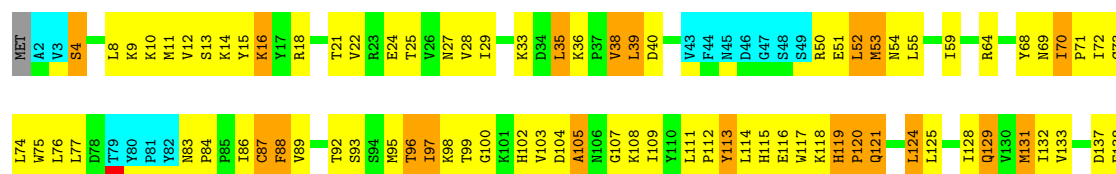


• Molecule 2: Gag Polyprotein



4.2.13 Score per residue for model 13

• Molecule 1: Tumor Susceptibility gene 101 protein

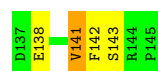
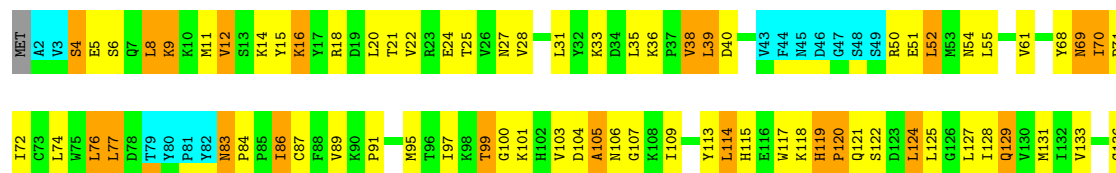
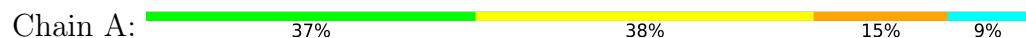


• Molecule 2: Gag Polyprotein

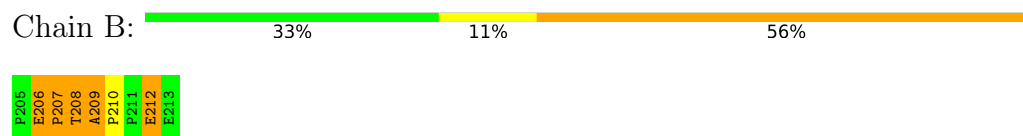


4.2.14 Score per residue for model 14

• Molecule 1: Tumor Susceptibility gene 101 protein

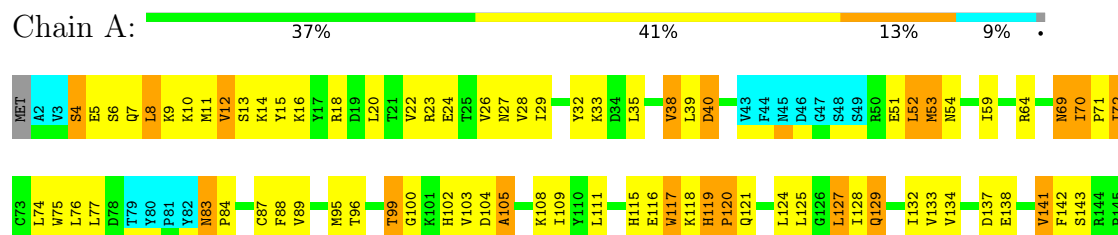


• Molecule 2: Gag Polyprotein

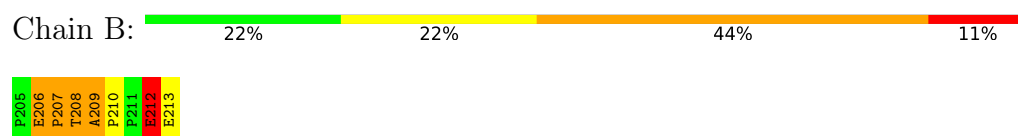


4.2.15 Score per residue for model 15

- Molecule 1: Tumor Susceptibility gene 101 protein

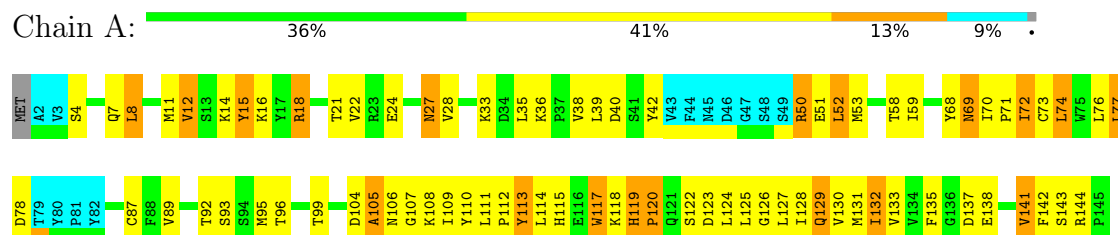


- Molecule 2: Gag Polyprotein

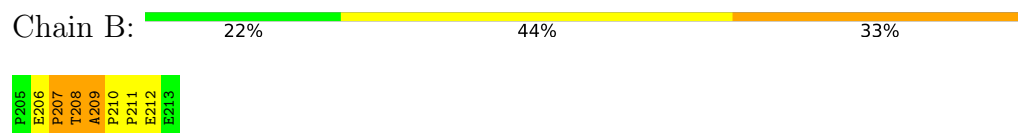


4.2.16 Score per residue for model 16

- Molecule 1: Tumor Susceptibility gene 101 protein

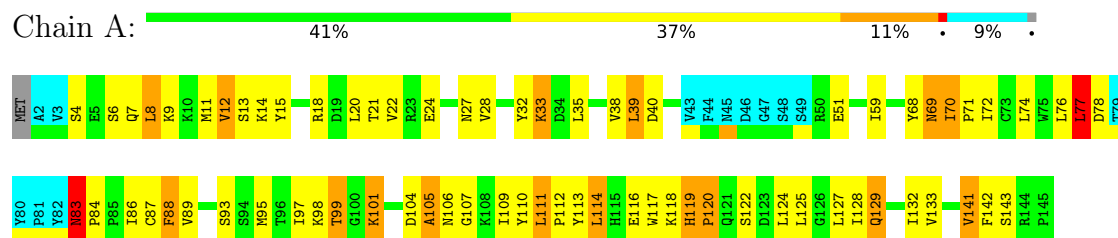


- Molecule 2: Gag Polyprotein

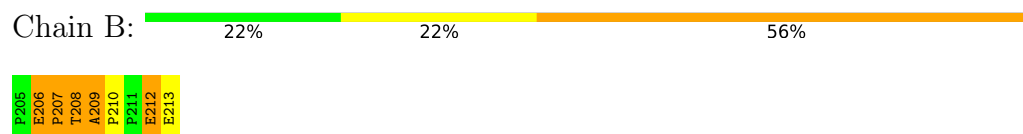


4.2.17 Score per residue for model 17

- Molecule 1: Tumor Susceptibility gene 101 protein

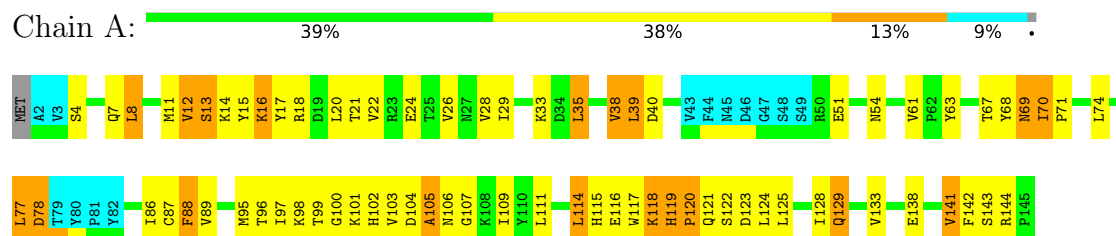


- Molecule 2: Gag Polyprotein



4.2.18 Score per residue for model 18

- Molecule 1: Tumor Susceptibility gene 101 protein

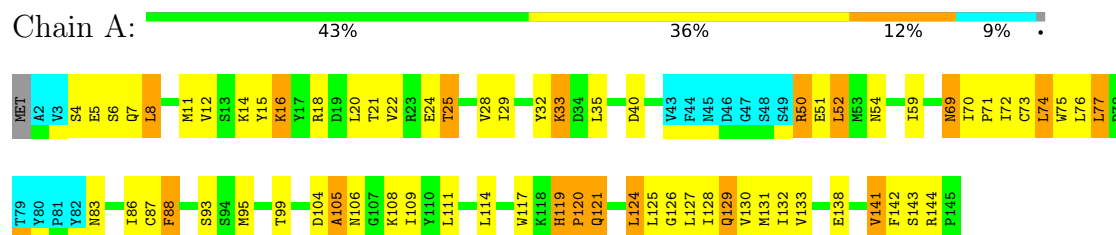


- Molecule 2: Gag Polyprotein

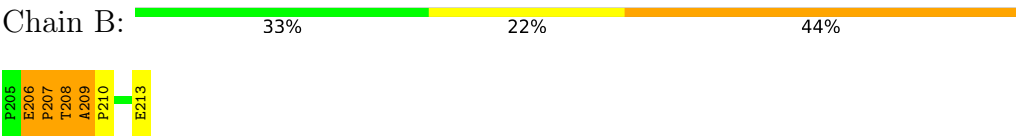


4.2.19 Score per residue for model 19

- Molecule 1: Tumor Susceptibility gene 101 protein

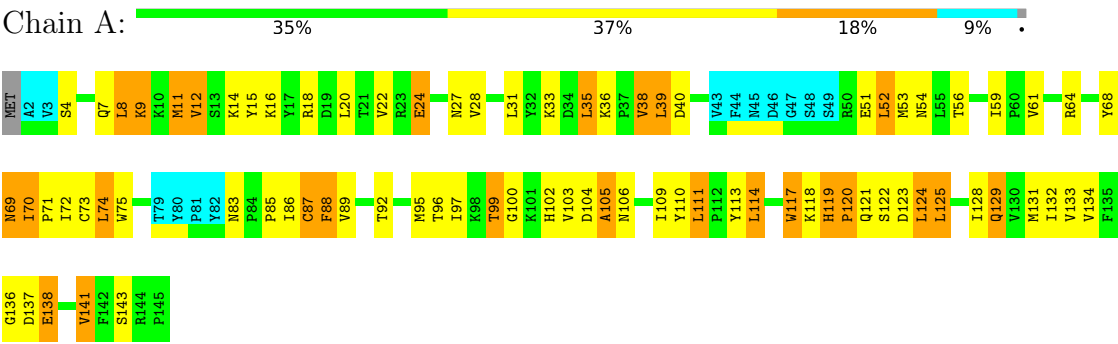


- Molecule 2: Gag Polyprotein

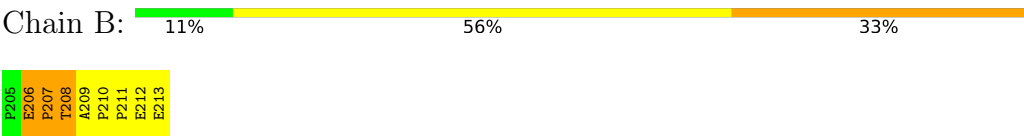


4.2.20 Score per residue for model 20

- 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 distance geometry simulated annealing*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
DYANA	structure solution	
CNS	refinement	

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	A	1062	1097	1094	60±9
2	B	68	60	58	18±3
All	All	22600	23140	23040	1329

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 29.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:LEU:HD11	1:A:124:LEU:HD11	0.92	1.41	5	5
1:A:95:MET:HE2	2:B:208:THR:C	0.84	1.97	15	18
1:A:102:HIS:CD2	1:A:111:LEU:HD12	0.83	2.08	6	1
1:A:89:VAL:HG12	1:A:107:GLY:O	0.83	1.73	13	11
1:A:59:ILE:HD12	1:A:72:ILE:HD12	0.82	1.50	7	2
1:A:71:PRO:O	1:A:89:VAL:HG23	0.80	1.76	6	12
1:A:99:THR:HG22	1:A:104:ASP:O	0.80	1.77	8	18
1:A:39:LEU:HD13	1:A:40:ASP:N	0.79	1.91	3	9
1:A:129:GLN:O	1:A:133:VAL:HG23	0.79	1.77	20	20
1:A:59:ILE:HD12	1:A:132:ILE:HG12	0.79	1.55	17	10
1:A:24:GLU:O	1:A:28:VAL:HG23	0.78	1.78	15	19
1:A:15:TYR:CD2	1:A:21:THR:HG21	0.78	2.13	10	14
1:A:92:THR:HG21	2:B:207:PRO:HG2	0.78	1.52	2	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:LEU:HD23	1:A:40:ASP:N	0.77	1.95	7	1
1:A:52:LEU:O	1:A:52:LEU:HD13	0.76	1.81	16	3
1:A:59:ILE:HD12	1:A:132:ILE:CG1	0.76	2.11	17	8
1:A:18:ARG:O	1:A:22:VAL:HG23	0.76	1.80	17	20
1:A:39:LEU:HD23	1:A:53:MET:HA	0.75	1.57	6	1
1:A:15:TYR:CE2	1:A:21:THR:HG21	0.74	2.17	2	7
1:A:11:MET:HE2	1:A:39:LEU:HD23	0.74	1.56	18	2
1:A:25:THR:CG2	1:A:53:MET:HE1	0.74	2.13	2	1
1:A:12:VAL:HG11	1:A:15:TYR:CD2	0.73	2.18	20	2
1:A:124:LEU:O	1:A:128:ILE:HD12	0.73	1.83	10	15
1:A:8:LEU:HD12	1:A:8:LEU:O	0.73	1.83	4	11
1:A:87:CYS:HB2	1:A:109:ILE:HD12	0.72	1.61	8	17
1:A:25:THR:HG21	1:A:53:MET:HE1	0.72	1.60	2	1
1:A:101:LYS:O	1:A:111:LEU:HD23	0.72	1.85	17	1
1:A:119:HIS:N	1:A:120:PRO:HA	0.72	2.00	8	20
1:A:87:CYS:CB	1:A:109:ILE:HD12	0.71	2.15	16	13
1:A:39:LEU:HD11	1:A:51:GLU:HG2	0.71	1.59	11	1
1:A:50:ARG:CD	1:A:52:LEU:HD12	0.71	2.16	3	1
1:A:111:LEU:HD21	1:A:113:TYR:CD2	0.70	2.21	13	2
1:A:141:VAL:O	2:B:209:ALA:HB1	0.70	1.86	6	20
1:A:53:MET:SD	1:A:76:LEU:HD22	0.70	2.26	12	1
1:A:59:ILE:HG22	1:A:70:ILE:HG22	0.70	1.62	13	1
1:A:109:ILE:HG21	1:A:113:TYR:OH	0.70	1.85	4	1
1:A:95:MET:HE1	2:B:207:PRO:HB2	0.70	1.63	2	10
2:B:208:THR:O	2:B:209:ALA:HB3	0.69	1.87	13	18
1:A:74:LEU:HD11	1:A:87:CYS:SG	0.69	2.27	7	3
1:A:8:LEU:HD21	1:A:25:THR:HG21	0.69	1.62	10	1
1:A:59:ILE:CD1	1:A:72:ILE:HD12	0.69	2.17	7	1
1:A:27:ASN:HB3	1:A:125:LEU:HD21	0.69	1.63	2	2
1:A:11:MET:HG2	1:A:39:LEU:HD23	0.69	1.65	4	4
1:A:95:MET:HG2	1:A:141:VAL:HG22	0.68	1.65	7	11
1:A:27:ASN:OD1	1:A:125:LEU:HD22	0.68	1.87	3	1
1:A:143:SER:HB3	2:B:208:THR:O	0.68	1.88	20	3
1:A:39:LEU:HD11	1:A:51:GLU:CG	0.68	2.18	11	1
1:A:128:ILE:HG22	1:A:132:ILE:HD11	0.68	1.65	19	10
1:A:141:VAL:O	2:B:209:ALA:CB	0.67	2.42	20	20
1:A:141:VAL:HG13	1:A:141:VAL:O	0.67	1.89	10	10
1:A:12:VAL:HG12	1:A:15:TYR:CE1	0.66	2.25	9	9
1:A:102:HIS:CD2	1:A:111:LEU:HD21	0.66	2.25	11	3
1:A:55:LEU:HD12	1:A:76:LEU:HD13	0.66	1.67	14	1
1:A:83:ASN:HB3	1:A:114:LEU:HD23	0.66	1.68	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:LEU:HD22	1:A:52:LEU:C	0.66	2.16	16	4
1:A:12:VAL:HG11	1:A:15:TYR:CE2	0.66	2.25	20	2
1:A:29:ILE:HG22	1:A:35:LEU:O	0.65	1.91	3	8
1:A:29:ILE:HG22	1:A:35:LEU:HB3	0.65	1.66	7	1
1:A:38:VAL:HG13	1:A:54:ASN:CG	0.65	2.17	8	7
1:A:12:VAL:HG12	1:A:15:TYR:CD1	0.65	2.27	2	8
1:A:141:VAL:O	1:A:141:VAL:HG13	0.65	1.91	20	10
1:A:53:MET:HE2	1:A:76:LEU:HD22	0.64	1.68	13	1
1:A:128:ILE:HG22	1:A:132:ILE:CD1	0.64	2.21	19	10
1:A:74:LEU:N	1:A:74:LEU:HD23	0.64	2.08	1	3
1:A:52:LEU:HD22	1:A:52:LEU:O	0.64	1.92	19	3
1:A:109:ILE:CD1	1:A:131:MET:HE2	0.64	2.22	11	5
1:A:35:LEU:HD13	1:A:59:ILE:HG23	0.64	1.70	8	1
1:A:87:CYS:HB3	1:A:109:ILE:HD12	0.63	1.70	4	2
1:A:11:MET:CG	1:A:39:LEU:HD23	0.63	2.23	4	1
1:A:114:LEU:HD23	1:A:118:LYS:HG3	0.63	1.71	17	2
1:A:25:THR:HG23	1:A:55:LEU:HD21	0.63	1.70	10	4
1:A:28:VAL:HG22	1:A:125:LEU:HD12	0.62	1.70	4	6
1:A:83:ASN:HB3	1:A:114:LEU:HD11	0.62	1.71	12	2
1:A:92:THR:HG21	2:B:207:PRO:CG	0.62	2.24	8	4
1:A:96:THR:C	1:A:141:VAL:HG23	0.62	2.19	11	6
1:A:35:LEU:HD13	1:A:59:ILE:HG12	0.62	1.72	20	1
1:A:52:LEU:HD21	1:A:77:LEU:HD22	0.62	1.71	14	1
1:A:111:LEU:HD13	1:A:112:PRO:HD2	0.61	1.72	17	1
1:A:95:MET:HE2	2:B:208:THR:O	0.61	1.94	5	15
2:B:208:THR:O	2:B:209:ALA:CB	0.61	2.48	18	18
1:A:12:VAL:HG12	1:A:15:TYR:CG	0.61	2.30	4	1
1:A:77:LEU:HD23	1:A:84:PRO:HA	0.61	1.72	17	1
1:A:97:ILE:HA	1:A:141:VAL:HG23	0.61	1.73	8	9
1:A:52:LEU:HD11	1:A:77:LEU:HD13	0.61	1.73	7	1
1:A:39:LEU:HD23	1:A:53:MET:CA	0.60	2.26	6	1
1:A:50:ARG:HD3	1:A:52:LEU:HD12	0.60	1.73	19	1
1:A:84:PRO:HG3	1:A:124:LEU:HD11	0.60	1.72	9	1
1:A:97:ILE:HG21	1:A:105:ALA:O	0.60	1.96	18	1
1:A:76:LEU:HD12	1:A:84:PRO:HG3	0.60	1.71	13	5
1:A:86:ILE:HG22	1:A:88:PHE:CZ	0.60	2.31	2	9
1:A:119:HIS:N	1:A:120:PRO:CA	0.60	2.64	10	20
1:A:9:LYS:HG3	1:A:22:VAL:HG21	0.60	1.72	12	6
1:A:37:PRO:HA	1:A:55:LEU:HD23	0.60	1.74	3	1
1:A:35:LEU:HD13	1:A:59:ILE:CG2	0.60	2.26	2	2
1:A:101:LYS:O	1:A:111:LEU:HD21	0.60	1.97	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:SER:HB2	2:B:208:THR:O	0.59	1.97	18	18
1:A:76:LEU:HD11	1:A:124:LEU:CD1	0.59	2.25	16	2
1:A:52:LEU:HD13	1:A:75:TRP:CE3	0.59	2.33	20	4
1:A:102:HIS:CD2	1:A:111:LEU:HD23	0.59	2.33	10	1
1:A:53:MET:HE2	1:A:76:LEU:CD2	0.59	2.27	13	2
1:A:74:LEU:HD21	1:A:131:MET:HE1	0.59	1.73	16	1
1:A:76:LEU:CD1	1:A:124:LEU:HD11	0.59	2.25	16	1
1:A:85:PRO:C	1:A:86:ILE:HG12	0.59	2.22	10	2
1:A:102:HIS:CE1	1:A:134:VAL:HG11	0.59	2.33	9	1
2:B:206:GLU:HB2	2:B:207:PRO:CD	0.58	2.28	7	20
1:A:89:VAL:HG12	1:A:107:GLY:CA	0.58	2.28	10	6
1:A:38:VAL:HG13	1:A:54:ASN:OD1	0.58	1.97	8	2
1:A:27:ASN:HB3	1:A:125:LEU:HD11	0.58	1.74	9	10
1:A:102:HIS:CD2	1:A:111:LEU:HD13	0.58	2.34	13	1
1:A:89:VAL:HG13	1:A:91:PRO:HD3	0.57	1.75	10	1
1:A:52:LEU:HD23	1:A:76:LEU:O	0.57	2.00	3	1
1:A:70:ILE:HD13	2:B:210:PRO:HD3	0.57	1.76	20	2
1:A:36:LYS:O	1:A:56:THR:HG22	0.57	1.99	1	3
1:A:25:THR:HG21	1:A:53:MET:CE	0.57	2.28	2	1
1:A:71:PRO:O	1:A:72:ILE:HD13	0.56	2.01	13	8
1:A:38:VAL:HG11	1:A:56:THR:HG22	0.56	1.78	2	1
1:A:96:THR:O	1:A:141:VAL:HG23	0.56	2.00	11	3
1:A:35:LEU:HD23	1:A:55:LEU:HD12	0.56	1.78	1	1
1:A:38:VAL:CG1	1:A:56:THR:HG22	0.56	2.31	2	2
1:A:39:LEU:HD23	1:A:40:ASP:H	0.56	1.59	7	1
1:A:83:ASN:HB3	1:A:114:LEU:HD21	0.56	1.78	17	1
1:A:38:VAL:HG13	1:A:54:ASN:ND2	0.56	2.16	10	6
1:A:72:ILE:HG23	1:A:73:CYS:N	0.56	2.15	2	4
1:A:25:THR:OG1	1:A:53:MET:HE1	0.55	2.02	2	1
1:A:143:SER:CB	2:B:208:THR:O	0.55	2.54	20	17
1:A:55:LEU:CD1	1:A:76:LEU:HD13	0.55	2.31	14	1
1:A:52:LEU:HD11	1:A:77:LEU:CD2	0.55	2.31	3	1
1:A:52:LEU:HD11	1:A:77:LEU:HD23	0.55	1.78	3	1
1:A:76:LEU:HD21	1:A:124:LEU:HD11	0.54	1.79	2	1
1:A:39:LEU:HD13	1:A:40:ASP:H	0.54	1.62	13	7
1:A:77:LEU:HD12	1:A:83:ASN:N	0.54	2.17	12	1
1:A:83:ASN:OD1	1:A:114:LEU:HD21	0.54	2.02	12	1
1:A:76:LEU:HD11	1:A:124:LEU:HD21	0.54	1.78	1	2
1:A:73:CYS:O	1:A:74:LEU:HD22	0.54	2.03	2	2
1:A:85:PRO:O	1:A:86:ILE:HD13	0.54	2.02	12	2
1:A:111:LEU:O	1:A:111:LEU:HD13	0.54	2.02	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:MET:HE2	1:A:76:LEU:HD23	0.54	1.79	15	1
1:A:100:GLY:O	1:A:101:LYS:CB	0.54	2.55	12	2
1:A:111:LEU:HD22	1:A:111:LEU:C	0.53	2.28	3	1
1:A:74:LEU:HD13	1:A:86:ILE:O	0.53	2.02	2	2
1:A:70:ILE:HG23	1:A:72:ILE:HD12	0.53	1.80	15	1
1:A:109:ILE:HD13	1:A:131:MET:SD	0.53	2.44	13	2
1:A:85:PRO:O	1:A:86:ILE:C	0.53	2.51	2	1
1:A:27:ASN:CB	1:A:125:LEU:HD11	0.53	2.34	9	3
1:A:91:PRO:HB3	1:A:141:VAL:HG21	0.53	1.80	8	2
1:A:95:MET:HE2	2:B:208:THR:CA	0.53	2.33	15	10
1:A:102:HIS:HD2	1:A:111:LEU:HD21	0.53	1.62	11	1
1:A:52:LEU:HD22	1:A:76:LEU:O	0.53	2.04	12	1
1:A:99:THR:HG21	1:A:104:ASP:O	0.52	2.05	5	1
1:A:111:LEU:HD22	1:A:112:PRO:N	0.52	2.20	3	1
1:A:8:LEU:CD2	1:A:25:THR:HG21	0.52	2.34	10	1
1:A:111:LEU:HB2	1:A:112:PRO:HD2	0.52	1.79	13	2
1:A:52:LEU:C	1:A:52:LEU:HD13	0.52	2.30	2	1
1:A:97:ILE:HD11	1:A:107:GLY:CA	0.52	2.35	2	1
1:A:71:PRO:HG3	1:A:95:MET:HE1	0.51	1.83	4	9
1:A:52:LEU:HD21	1:A:77:LEU:HD12	0.51	1.80	13	2
1:A:35:LEU:HD21	1:A:59:ILE:HG23	0.51	1.83	11	1
2:B:208:THR:CG2	2:B:209:ALA:N	0.51	2.74	13	18
1:A:24:GLU:HB3	1:A:124:LEU:HD22	0.51	1.82	4	2
1:A:70:ILE:HD13	2:B:210:PRO:CD	0.51	2.35	20	2
1:A:11:MET:HB3	1:A:39:LEU:HD23	0.51	1.83	8	2
1:A:83:ASN:CB	1:A:114:LEU:HD21	0.50	2.36	17	1
1:A:39:LEU:HD11	1:A:51:GLU:HB2	0.50	1.83	4	1
1:A:52:LEU:HD22	1:A:75:TRP:CE3	0.50	2.41	7	1
2:B:208:THR:HG22	2:B:209:ALA:N	0.50	2.22	12	6
1:A:74:LEU:H	1:A:74:LEU:HD23	0.50	1.66	17	6
1:A:55:LEU:CD2	1:A:76:LEU:HD22	0.50	2.36	4	1
1:A:11:MET:HE3	1:A:39:LEU:HD23	0.50	1.83	20	1
1:A:111:LEU:HD13	1:A:112:PRO:CD	0.50	2.36	17	1
1:A:113:TYR:CE2	1:A:114:LEU:HD12	0.50	2.42	3	1
1:A:83:ASN:CG	1:A:114:LEU:HD11	0.50	2.32	10	1
1:A:50:ARG:NH2	1:A:77:LEU:HD21	0.50	2.22	19	2
1:A:86:ILE:CG2	1:A:88:PHE:CE2	0.50	2.95	11	12
1:A:117:TRP:CH2	1:A:119:HIS:CD2	0.50	3.00	16	2
1:A:59:ILE:HD11	1:A:132:ILE:HD11	0.50	1.83	13	1
1:A:50:ARG:NH1	1:A:77:LEU:HD12	0.50	2.22	11	1
1:A:14:LYS:O	1:A:15:TYR:CD1	0.50	2.65	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:VAL:C	1:A:67:THR:HG23	0.50	2.32	18	1
1:A:97:ILE:CA	1:A:141:VAL:HG23	0.49	2.37	10	5
1:A:111:LEU:CB	1:A:112:PRO:HD2	0.49	2.37	13	2
1:A:8:LEU:HD21	1:A:25:THR:HB	0.49	1.83	19	2
1:A:8:LEU:HD21	1:A:25:THR:CG2	0.49	2.35	10	1
1:A:32:TYR:O	1:A:33:LYS:CG	0.49	2.60	4	6
1:A:96:THR:O	1:A:97:ILE:HG12	0.49	2.07	13	1
1:A:113:TYR:CD2	1:A:114:LEU:HD12	0.49	2.42	3	1
1:A:85:PRO:HD2	1:A:86:ILE:HD12	0.49	1.84	20	1
1:A:9:LYS:O	1:A:12:VAL:HG23	0.49	2.07	15	7
1:A:11:MET:HG2	1:A:39:LEU:HD13	0.49	1.84	7	1
1:A:12:VAL:HG12	1:A:15:TYR:CD2	0.49	2.42	4	1
1:A:86:ILE:CG2	1:A:88:PHE:CZ	0.49	2.96	2	9
1:A:8:LEU:HD12	1:A:8:LEU:C	0.48	2.33	2	8
1:A:28:VAL:HG22	1:A:125:LEU:HD22	0.48	1.83	5	1
1:A:104:ASP:O	1:A:105:ALA:HB2	0.48	2.09	16	20
1:A:39:LEU:C	1:A:39:LEU:HD13	0.48	2.34	9	2
1:A:69:ASN:O	2:B:207:PRO:HA	0.48	2.08	7	1
1:A:52:LEU:CD2	1:A:54:ASN:OD1	0.48	2.61	11	2
1:A:50:ARG:CZ	1:A:77:LEU:HD21	0.48	2.39	19	1
1:A:95:MET:HE2	2:B:209:ALA:CB	0.48	2.39	20	1
1:A:61:VAL:HG13	1:A:136:GLY:HA2	0.48	1.85	20	2
1:A:52:LEU:HD11	1:A:77:LEU:CD1	0.47	2.38	7	1
1:A:83:ASN:CB	1:A:114:LEU:HD11	0.47	2.39	12	2
1:A:8:LEU:O	1:A:11:MET:HG2	0.47	2.09	18	1
1:A:11:MET:SD	1:A:39:LEU:HD23	0.47	2.49	11	1
1:A:69:ASN:ND2	2:B:206:GLU:O	0.47	2.47	12	18
1:A:114:LEU:HD13	1:A:114:LEU:O	0.47	2.09	4	1
1:A:74:LEU:HD23	1:A:74:LEU:N	0.47	2.24	17	4
1:A:15:TYR:HD2	1:A:21:THR:HG21	0.47	1.69	9	3
1:A:38:VAL:HG22	1:A:54:ASN:O	0.47	2.09	12	1
1:A:14:LYS:CG	1:A:14:LYS:O	0.47	2.63	16	1
1:A:85:PRO:O	1:A:86:ILE:O	0.47	2.33	2	1
1:A:113:TYR:CD1	1:A:114:LEU:N	0.47	2.83	17	1
1:A:99:THR:CG2	1:A:104:ASP:O	0.47	2.63	2	1
1:A:8:LEU:C	1:A:8:LEU:HD12	0.47	2.35	12	2
1:A:68:TYR:CZ	2:B:211:PRO:CD	0.47	2.98	12	4
1:A:86:ILE:HG22	1:A:88:PHE:CE2	0.47	2.45	8	3
1:A:59:ILE:O	1:A:70:ILE:N	0.47	2.46	16	1
1:A:52:LEU:HD21	1:A:75:TRP:CE3	0.47	2.44	19	1
1:A:73:CYS:C	1:A:74:LEU:HD23	0.47	2.35	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:VAL:CG1	1:A:15:TYR:CD1	0.47	2.98	17	6
1:A:142:PHE:CD1	1:A:142:PHE:O	0.47	2.68	18	1
1:A:12:VAL:CG1	1:A:15:TYR:CE2	0.46	2.98	20	2
1:A:50:ARG:HH11	1:A:52:LEU:HD12	0.46	1.69	7	1
1:A:71:PRO:HG3	1:A:95:MET:HE2	0.46	1.86	11	1
1:A:141:VAL:O	1:A:141:VAL:CG1	0.46	2.60	2	11
1:A:8:LEU:HD23	1:A:26:VAL:HG12	0.46	1.87	18	2
1:A:39:LEU:HD12	1:A:53:MET:HG3	0.46	1.87	7	1
1:A:88:PHE:CD1	1:A:88:PHE:N	0.46	2.84	2	2
1:A:72:ILE:HG22	1:A:73:CYS:N	0.46	2.25	8	7
1:A:15:TYR:CD1	1:A:15:TYR:C	0.46	2.94	7	1
1:A:86:ILE:HG23	1:A:88:PHE:CZ	0.46	2.46	9	1
1:A:114:LEU:HD23	1:A:118:LYS:HB3	0.46	1.88	20	1
1:A:12:VAL:HG11	1:A:15:TYR:CD1	0.46	2.46	7	1
1:A:35:LEU:CD1	1:A:59:ILE:HG23	0.46	2.41	8	1
1:A:85:PRO:O	1:A:86:ILE:CD1	0.46	2.64	10	2
1:A:86:ILE:HG22	1:A:87:CYS:N	0.46	2.26	4	1
1:A:53:MET:CE	1:A:76:LEU:HD23	0.46	2.41	11	1
2:B:207:PRO:O	2:B:209:ALA:N	0.45	2.48	17	19
1:A:100:GLY:O	1:A:101:LYS:HB2	0.45	2.10	12	2
1:A:52:LEU:C	1:A:52:LEU:CD2	0.45	2.89	11	3
1:A:84:PRO:CB	1:A:127:LEU:HD11	0.45	2.41	15	1
1:A:100:GLY:O	1:A:103:VAL:O	0.45	2.34	7	10
1:A:127:LEU:C	1:A:127:LEU:HD23	0.45	2.36	17	1
1:A:52:LEU:HD21	1:A:54:ASN:OD1	0.45	2.12	19	1
1:A:76:LEU:HD21	1:A:124:LEU:CD1	0.45	2.41	2	1
1:A:70:ILE:O	1:A:70:ILE:CG2	0.45	2.64	20	5
1:A:59:ILE:HG13	1:A:60:PRO:HD2	0.45	1.86	6	1
1:A:75:TRP:CD1	1:A:88:PHE:CE1	0.45	3.05	11	1
1:A:40:ASP:CG	1:A:75:TRP:CZ3	0.45	2.94	9	1
1:A:87:CYS:O	1:A:88:PHE:CD1	0.45	2.69	9	1
1:A:11:MET:CE	1:A:39:LEU:HD23	0.45	2.41	1	2
1:A:111:LEU:CB	1:A:112:PRO:CD	0.45	2.94	13	2
1:A:52:LEU:CD1	1:A:75:TRP:CE3	0.45	2.99	2	1
1:A:31:LEU:HD22	1:A:125:LEU:CD2	0.45	2.42	20	1
1:A:83:ASN:HB2	1:A:114:LEU:HD11	0.45	1.87	1	1
1:A:38:VAL:CG2	1:A:39:LEU:N	0.45	2.80	7	1
1:A:70:ILE:CD1	2:B:210:PRO:HD3	0.45	2.42	13	9
1:A:111:LEU:CD2	1:A:113:TYR:CD2	0.45	2.99	13	1
1:A:28:VAL:CG2	1:A:125:LEU:HD12	0.45	2.42	4	2
1:A:16:LYS:CD	1:A:17:TYR:CZ	0.45	3.00	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:LEU:HD12	1:A:114:LEU:N	0.45	2.27	19	1
1:A:54:ASN:OD1	1:A:54:ASN:N	0.44	2.49	12	3
1:A:84:PRO:HB3	1:A:127:LEU:HD11	0.44	1.90	4	1
1:A:89:VAL:HG12	1:A:107:GLY:C	0.44	2.37	10	4
1:A:21:THR:HG22	1:A:53:MET:HE1	0.44	1.89	7	1
2:B:207:PRO:C	2:B:209:ALA:H	0.44	2.20	8	2
1:A:92:THR:CG2	2:B:207:PRO:HG2	0.44	2.43	1	5
1:A:142:PHE:CB	2:B:210:PRO:O	0.44	2.65	7	9
1:A:52:LEU:HD22	1:A:53:MET:O	0.44	2.12	16	1
1:A:126:GLY:O	1:A:130:VAL:HG23	0.44	2.12	19	2
1:A:111:LEU:O	1:A:113:TYR:CD2	0.44	2.71	17	1
2:B:206:GLU:CB	2:B:207:PRO:CD	0.44	2.94	7	16
1:A:29:ILE:CG2	1:A:55:LEU:HD22	0.44	2.42	2	1
1:A:117:TRP:CZ2	1:A:119:HIS:CD2	0.44	3.06	6	1
1:A:109:ILE:HD11	1:A:131:MET:SD	0.44	2.53	1	2
1:A:77:LEU:N	1:A:77:LEU:HD22	0.44	2.28	7	1
1:A:73:CYS:O	1:A:88:PHE:CD1	0.44	2.70	10	2
1:A:103:VAL:HG12	1:A:108:LYS:O	0.44	2.13	12	1
1:A:95:MET:HG2	1:A:141:VAL:CG2	0.44	2.41	8	2
1:A:31:LEU:HD22	1:A:125:LEU:HD23	0.44	1.88	14	2
1:A:12:VAL:CG1	1:A:15:TYR:CD2	0.44	2.98	1	3
1:A:15:TYR:HE2	1:A:21:THR:HG21	0.44	1.68	2	1
1:A:77:LEU:HD12	1:A:77:LEU:C	0.44	2.38	6	1
1:A:12:VAL:CG1	1:A:15:TYR:CE1	0.44	3.00	9	3
1:A:70:ILE:CD1	2:B:210:PRO:CD	0.43	2.96	8	7
1:A:96:THR:HG22	1:A:142:PHE:O	0.43	2.13	15	1
1:A:73:CYS:N	1:A:88:PHE:O	0.43	2.52	4	1
1:A:77:LEU:HD12	1:A:83:ASN:C	0.43	2.38	12	2
1:A:32:TYR:CE1	1:A:132:ILE:CD1	0.43	3.01	15	1
1:A:112:PRO:O	1:A:114:LEU:N	0.43	2.52	2	1
1:A:55:LEU:HD23	1:A:76:LEU:HD22	0.43	1.89	4	1
1:A:83:ASN:CB	1:A:84:PRO:CD	0.43	2.96	11	1
1:A:12:VAL:O	1:A:14:LYS:N	0.43	2.49	4	1
1:A:28:VAL:HG21	1:A:124:LEU:HD23	0.43	1.89	13	1
1:A:74:LEU:N	1:A:74:LEU:CD2	0.43	2.80	20	3
1:A:117:TRP:CD1	1:A:120:PRO:O	0.43	2.72	15	2
1:A:53:MET:HE1	1:A:76:LEU:CD2	0.43	2.43	11	1
1:A:89:VAL:HG12	1:A:107:GLY:HA2	0.43	1.88	4	1
1:A:25:THR:CG2	1:A:55:LEU:HD21	0.43	2.44	9	1
1:A:75:TRP:CD1	1:A:88:PHE:CZ	0.43	3.07	11	1
1:A:52:LEU:HD21	1:A:78:ASP:OD1	0.43	2.14	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:VAL:HG23	1:A:13:SER:H	0.43	1.72	18	1
1:A:111:LEU:HD13	1:A:111:LEU:C	0.43	2.38	3	1
1:A:5:GLU:OE2	1:A:29:ILE:HD11	0.43	2.14	12	1
1:A:15:TYR:O	1:A:16:LYS:C	0.43	2.62	7	1
1:A:7:GLN:O	1:A:10:LYS:CG	0.43	2.67	9	1
1:A:74:LEU:HD23	1:A:74:LEU:H	0.43	1.72	15	2
1:A:128:ILE:HA	1:A:131:MET:HG3	0.43	1.90	8	1
1:A:32:TYR:CE1	1:A:132:ILE:HD13	0.43	2.49	15	1
1:A:52:LEU:HD21	1:A:75:TRP:HE3	0.43	1.74	15	1
1:A:35:LEU:HD21	1:A:59:ILE:CG2	0.43	2.44	11	1
1:A:97:ILE:CG2	1:A:98:LYS:N	0.43	2.82	17	2
1:A:37:PRO:CA	1:A:55:LEU:HD23	0.42	2.42	3	1
1:A:63:TYR:O	1:A:64:ARG:CB	0.42	2.66	11	1
1:A:86:ILE:HG21	1:A:88:PHE:CE2	0.42	2.48	11	1
1:A:38:VAL:HG22	1:A:54:ASN:ND2	0.42	2.29	15	1
1:A:70:ILE:O	1:A:70:ILE:HG23	0.42	2.14	4	1
1:A:38:VAL:HG22	1:A:39:LEU:N	0.42	2.28	7	1
1:A:99:THR:HA	1:A:103:VAL:HG23	0.42	1.90	12	1
1:A:114:LEU:HD12	1:A:118:LYS:HD2	0.42	1.91	12	1
1:A:102:HIS:CD2	1:A:111:LEU:HD11	0.42	2.49	4	2
1:A:95:MET:CE	2:B:208:THR:N	0.42	2.82	7	4
1:A:62:PRO:HA	1:A:67:THR:HA	0.42	1.91	2	1
1:A:92:THR:CG2	2:B:207:PRO:CG	0.42	2.97	7	1
1:A:15:TYR:CE2	1:A:77:LEU:O	0.42	2.72	12	3
1:A:68:TYR:CE1	2:B:211:PRO:HD3	0.42	2.50	20	2
1:A:83:ASN:CB	1:A:84:PRO:HD3	0.42	2.44	15	1
1:A:77:LEU:H	1:A:77:LEU:HD22	0.42	1.75	11	1
1:A:26:VAL:HG23	1:A:27:ASN:N	0.42	2.30	15	2
1:A:68:TYR:CZ	2:B:211:PRO:HD3	0.42	2.50	18	3
1:A:120:PRO:O	1:A:121:GLN:CB	0.42	2.67	13	4
1:A:128:ILE:HD12	1:A:128:ILE:H	0.42	1.74	17	2
1:A:38:VAL:CG1	1:A:54:ASN:ND2	0.42	2.83	10	1
1:A:102:HIS:C	1:A:103:VAL:CG2	0.42	2.92	11	3
1:A:131:MET:O	1:A:135:PHE:CD2	0.42	2.72	4	2
1:A:95:MET:HE2	2:B:208:THR:N	0.42	2.30	7	1
1:A:84:PRO:O	1:A:114:LEU:HD11	0.42	2.15	11	1
1:A:102:HIS:CG	1:A:138:GLU:OE1	0.42	2.72	11	1
1:A:142:PHE:CD1	2:B:212:GLU:HG3	0.42	2.49	18	1
1:A:59:ILE:CG1	1:A:70:ILE:HG22	0.42	2.44	19	2
1:A:131:MET:O	1:A:135:PHE:CG	0.42	2.73	8	1
1:A:85:PRO:C	1:A:86:ILE:CG1	0.42	2.93	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:MET:HE3	2:B:209:ALA:HB2	0.42	1.90	11	1
1:A:142:PHE:CE1	2:B:212:GLU:OE1	0.42	2.73	7	7
1:A:111:LEU:O	1:A:113:TYR:N	0.42	2.52	3	1
1:A:59:ILE:CG2	1:A:70:ILE:HG22	0.42	2.45	6	1
1:A:76:LEU:HD21	1:A:124:LEU:HD21	0.42	1.91	7	1
1:A:97:ILE:HD13	1:A:107:GLY:N	0.42	2.29	14	1
1:A:70:ILE:CG2	1:A:72:ILE:HD12	0.42	2.45	15	1
1:A:102:HIS:CE1	1:A:134:VAL:CG1	0.42	3.03	15	1
1:A:117:TRP:O	1:A:118:LYS:CG	0.41	2.68	7	3
1:A:83:ASN:H	1:A:84:PRO:CD	0.41	2.28	4	1
1:A:27:ASN:CG	1:A:125:LEU:HD22	0.41	2.38	3	1
1:A:76:LEU:HD11	1:A:124:LEU:CD2	0.41	2.44	3	1
2:B:206:GLU:HB2	2:B:207:PRO:HD2	0.41	1.93	11	4
1:A:4:SER:O	1:A:8:LEU:N	0.41	2.53	14	3
1:A:16:LYS:HB2	1:A:78:ASP:HA	0.41	1.92	7	1
1:A:77:LEU:HD23	1:A:84:PRO:CA	0.41	2.45	17	1
1:A:114:LEU:HD23	1:A:118:LYS:CG	0.41	2.43	17	1
1:A:97:ILE:N	1:A:141:VAL:HG23	0.41	2.30	10	3
1:A:102:HIS:CD2	1:A:134:VAL:HG11	0.41	2.50	7	1
1:A:113:TYR:CD2	1:A:114:LEU:N	0.41	2.89	8	1
1:A:75:TRP:O	1:A:85:PRO:CG	0.41	2.69	11	1
1:A:99:THR:HG21	1:A:105:ALA:HA	0.41	1.92	12	1
1:A:15:TYR:CD1	1:A:15:TYR:O	0.41	2.73	7	1
1:A:68:TYR:CZ	2:B:211:PRO:HD2	0.41	2.51	16	1
1:A:40:ASP:CB	1:A:54:ASN:ND2	0.41	2.83	19	1
1:A:63:TYR:CE2	2:B:211:PRO:O	0.41	2.73	18	2
1:A:104:ASP:OD2	1:A:110:TYR:CG	0.41	2.74	17	1
1:A:15:TYR:CD1	1:A:78:ASP:HA	0.41	2.50	18	1
1:A:32:TYR:O	1:A:33:LYS:HG3	0.41	2.16	19	1
1:A:68:TYR:CD2	2:B:209:ALA:O	0.41	2.74	1	6
1:A:83:ASN:HB3	1:A:84:PRO:HD3	0.41	1.93	11	3
1:A:110:TYR:CD2	1:A:110:TYR:O	0.41	2.74	16	1
1:A:72:ILE:CG2	1:A:73:CYS:N	0.41	2.84	3	1
1:A:29:ILE:O	1:A:33:LYS:N	0.41	2.52	9	2
1:A:72:ILE:HG22	1:A:73:CYS:H	0.41	1.76	7	1
1:A:84:PRO:CG	1:A:124:LEU:HD11	0.41	2.43	9	1
1:A:102:HIS:CE1	1:A:138:GLU:OE1	0.41	2.74	18	2
1:A:28:VAL:CG2	1:A:124:LEU:HD23	0.41	2.46	13	1
1:A:142:PHE:CE1	2:B:212:GLU:OE2	0.41	2.73	15	1
1:A:50:ARG:HD2	1:A:52:LEU:HD12	0.41	1.93	3	1
1:A:38:VAL:HG13	1:A:54:ASN:O	0.41	2.16	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:TYR:CG	1:A:63:TYR:O	0.41	2.74	6	1
1:A:77:LEU:HD12	1:A:83:ASN:O	0.41	2.15	10	1
1:A:111:LEU:HD22	1:A:112:PRO:C	0.41	2.41	3	1
1:A:111:LEU:HB2	1:A:112:PRO:CD	0.41	2.46	13	1
1:A:117:TRP:O	1:A:118:LYS:HG3	0.40	2.15	2	1
1:A:102:HIS:CD2	1:A:111:LEU:HG	0.40	2.51	9	1
1:A:114:LEU:HD12	1:A:118:LYS:CD	0.40	2.46	12	1
1:A:114:LEU:N	1:A:114:LEU:CD1	0.40	2.83	19	1
1:A:102:HIS:ND1	1:A:111:LEU:CD1	0.40	2.84	20	2
1:A:15:TYR:O	1:A:17:TYR:N	0.40	2.53	7	1
1:A:117:TRP:NE1	1:A:120:PRO:O	0.40	2.55	7	1
1:A:53:MET:CE	1:A:76:LEU:CD2	0.40	3.00	11	1
1:A:109:ILE:HD13	1:A:131:MET:HE2	0.40	1.92	11	1
1:A:40:ASP:OD2	1:A:75:TRP:CZ3	0.40	2.74	15	1
1:A:15:TYR:CD1	1:A:78:ASP:OD1	0.40	2.75	5	1
1:A:55:LEU:N	1:A:55:LEU:CD2	0.40	2.84	7	1
1:A:95:MET:CG	1:A:141:VAL:HG22	0.40	2.46	16	2
1:A:111:LEU:HD12	1:A:113:TYR:CD1	0.40	2.51	10	1
1:A:40:ASP:OD2	1:A:75:TRP:CH2	0.40	2.75	11	1
1:A:74:LEU:CD2	1:A:131:MET:HE1	0.40	2.45	16	1
1:A:50:ARG:NE	1:A:52:LEU:HD12	0.40	2.31	3	1
1:A:131:MET:CG	1:A:135:PHE:CZ	0.40	3.04	6	1
1:A:91:PRO:HG3	1:A:97:ILE:HD11	0.40	1.90	14	1
1:A:134:VAL:O	1:A:138:GLU:CG	0.40	2.70	20	1
1:A:17:TYR:O	1:A:21:THR:N	0.40	2.52	18	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	130/145 (90%)	109±3 (84±2%)	16±2 (12±2%)	5±2 (4±1%)	3	28
2	B	7/9 (78%)	2±0 (31±5%)	3±1 (41±8%)	2±0 (28±5%)	0	1
All	All	2740/3080 (89%)	2216 (81%)	376 (14%)	148 (5%)	2	22

All 18 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	105	ALA	20
1	A	120	PRO	20
2	B	207	PRO	20
1	A	117	TRP	19
1	A	141	VAL	18
2	B	209	ALA	17
1	A	83	ASN	9
1	A	113	TYR	4
1	A	85	PRO	4
1	A	77	LEU	3
1	A	78	ASP	3
1	A	86	ILE	2
1	A	93	SER	2
1	A	101	LYS	2
2	B	212	GLU	2
1	A	100	GLY	1
1	A	16	LYS	1
1	A	65	GLY	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	124/136 (91%)	88±5 (71±4%)	36±5 (29±4%)	1	19
2	B	8/8 (100%)	5±1 (57±7%)	3±1 (42±7%)	0	4
All	All	2640/2880 (92%)	1857 (70%)	783 (30%)	1	17

All 86 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	8	LEU	20
1	A	12	VAL	20
1	A	69	ASN	20
1	A	119	HIS	20

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Mol	Chain	Res	Type	Models (Total)
1	A	129	GLN	20
2	B	208	THR	20
1	A	33	LYS	19
2	B	212	GLU	19
1	A	51	GLU	18
2	B	206	GLU	18
1	A	38	VAL	17
1	A	106	ASN	17
1	A	121	GLN	17
1	A	4	SER	16
1	A	16	LYS	15
1	A	20	LEU	15
1	A	35	LEU	15
1	A	114	LEU	15
1	A	122	SER	15
1	A	7	GLN	14
1	A	88	PHE	14
1	A	124	LEU	14
1	A	52	LEU	13
1	A	36	LYS	13
1	A	11	MET	12
1	A	39	LEU	12
1	A	138	GLU	12
1	A	76	LEU	12
1	A	77	LEU	12
1	A	74	LEU	11
1	A	96	THR	11
1	A	115	HIS	11
2	B	213	GLU	11
1	A	50	ARG	10
1	A	13	SER	10
1	A	14	LYS	10
1	A	70	ILE	10
1	A	118	LYS	10
1	A	127	LEU	10
1	A	6	SER	10
1	A	99	THR	9
1	A	101	LYS	9
1	A	108	LYS	9
1	A	137	ASP	9
1	A	5	GLU	8
1	A	125	LEU	8

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Mol	Chain	Res	Type	Models (Total)
1	A	116	GLU	8
1	A	83	ASN	7
1	A	111	LEU	7
1	A	23	ARG	7
1	A	93	SER	7
1	A	64	ARG	7
1	A	144	ARG	7
1	A	18	ARG	6
1	A	72	ILE	6
1	A	9	LYS	5
1	A	87	CYS	5
1	A	90	LYS	5
1	A	123	ASP	5
1	A	24	GLU	5
1	A	10	LYS	5
1	A	19	ASP	4
1	A	131	MET	4
1	A	53	MET	4
1	A	40	ASP	4
1	A	94	SER	4
1	A	27	ASN	3
1	A	55	LEU	3
1	A	97	ILE	3
1	A	15	TYR	3
1	A	25	THR	3
1	A	86	ILE	3
1	A	98	LYS	3
1	A	113	TYR	3
1	A	67	THR	2
1	A	34	ASP	2
1	A	66	ASN	2
1	A	78	ASP	2
1	A	103	VAL	2
1	A	32	TYR	1
1	A	54	ASN	1
1	A	59	ILE	1
1	A	95	MET	1
1	A	58	THR	1
1	A	132	ILE	1
1	A	110	TYR	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided