Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 06:48 PM EDT

PDB ID	:	2RNM
Title	:	Structure of The HET-s(218-289) prion in its amyloid form obtained by solid-state NMR
Authors	:	Wasmer, C.; Lange, A.; Van Melckebeke, H.; Siemer, A.; Riek, R.; Meier, B.H.
Deposited on	:	2008-01-24

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 (i) 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 (i)) were used in the production of this report:

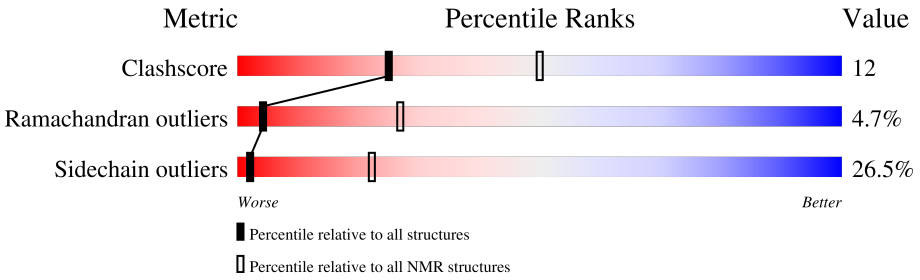
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	79	38% 25% 37%
1	B	79	37% 32% 32%
1	C	79	38% 29% • 32%
1	D	79	38% 29% 33%
1	E	79	35% 24% 41%

2 Ensemble composition and analysis

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:225-A:246, A:260-A:287, B:225-B:249, B:259-B:287, C:225-C:249, C:259-C:287, D:225-D:249, D:260-D:287, E:225-E:249, E:261-E:282 (258)	1.25	19

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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6014 atoms, of which 2969 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Small s protein.

Mol	Chain	Residues	Atoms						Trace
1	A	79	Total	C	H	N	O	S	0
			1202	371	593	123	114	1	
1	B	79	Total	C	H	N	O	S	0
			1203	371	594	123	114	1	
1	C	79	Total	C	H	N	O	S	0
			1203	371	594	123	114	1	
1	D	79	Total	C	H	N	O	S	0
			1203	371	594	123	114	1	
1	E	79	Total	C	H	N	O	S	0
			1203	371	594	123	114	1	

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	MET	-	initiating methionine	UNP Q03689
A	290	HIS	-	expression tag	UNP Q03689
A	291	HIS	-	expression tag	UNP Q03689
A	292	HIS	-	expression tag	UNP Q03689
A	293	HIS	-	expression tag	UNP Q03689
A	294	HIS	-	expression tag	UNP Q03689
A	295	HIS	-	expression tag	UNP Q03689
B	217	MET	-	initiating methionine	UNP Q03689
B	290	HIS	-	expression tag	UNP Q03689
B	291	HIS	-	expression tag	UNP Q03689
B	292	HIS	-	expression tag	UNP Q03689
B	293	HIS	-	expression tag	UNP Q03689
B	294	HIS	-	expression tag	UNP Q03689
B	295	HIS	-	expression tag	UNP Q03689
C	217	MET	-	initiating methionine	UNP Q03689
C	290	HIS	-	expression tag	UNP Q03689
C	291	HIS	-	expression tag	UNP Q03689
C	292	HIS	-	expression tag	UNP Q03689
C	293	HIS	-	expression tag	UNP Q03689
C	294	HIS	-	expression tag	UNP Q03689
C	295	HIS	-	expression tag	UNP Q03689
D	217	MET	-	initiating methionine	UNP Q03689
D	290	HIS	-	expression tag	UNP Q03689

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Chain	Residue	Modelled	Actual	Comment	Reference
D	291	HIS	-	expression tag	UNP Q03689
D	292	HIS	-	expression tag	UNP Q03689
D	293	HIS	-	expression tag	UNP Q03689
D	294	HIS	-	expression tag	UNP Q03689
D	295	HIS	-	expression tag	UNP Q03689
E	217	MET	-	initiating methionine	UNP Q03689
E	290	HIS	-	expression tag	UNP Q03689
E	291	HIS	-	expression tag	UNP Q03689
E	292	HIS	-	expression tag	UNP Q03689
E	293	HIS	-	expression tag	UNP Q03689
E	294	HIS	-	expression tag	UNP Q03689
E	295	HIS	-	expression tag	UNP Q03689

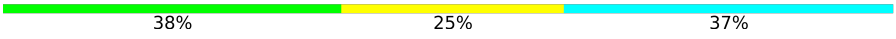
4 Residue-property plots

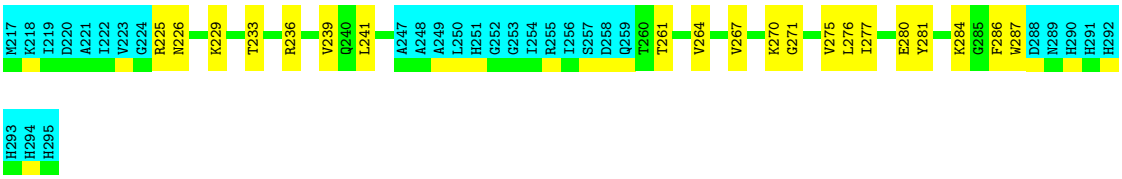
4.1 Average score per residue in the NMR ensemble

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: Small s protein

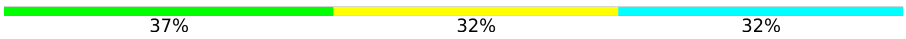
Chain A:

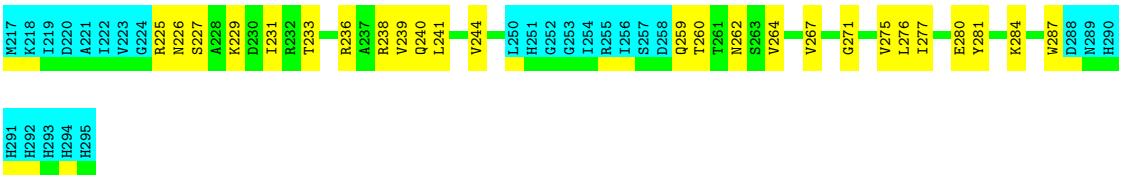




• Molecule 1: Small s protein

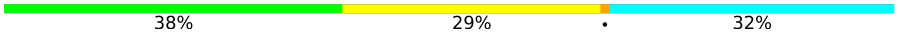
Chain B:

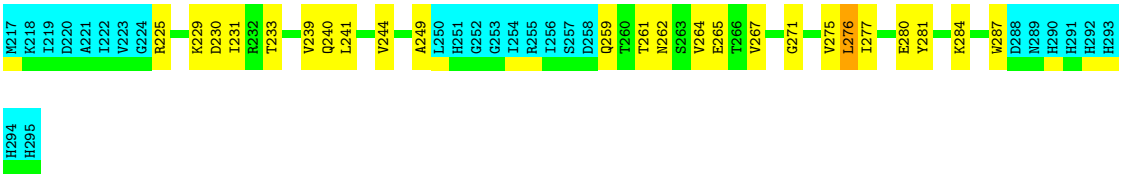




• Molecule 1: Small s protein

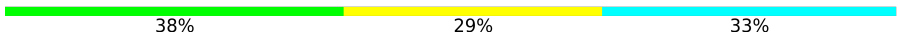
Chain C:





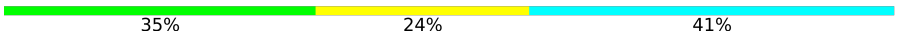
• Molecule 1: Small s protein

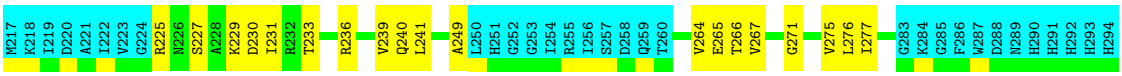
Chain D:



• Molecule 1: Small s protein

Chain E:





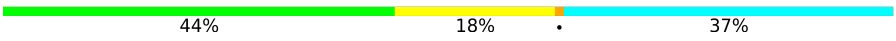
4.2 Scores per residue for each member of the ensemble

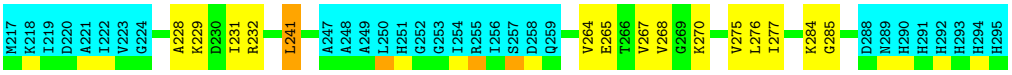
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Small s protein

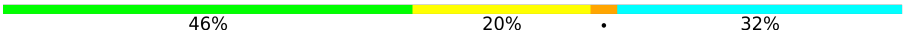
Chain A:

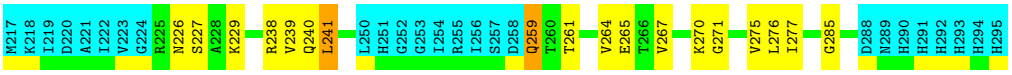




• Molecule 1: Small s protein

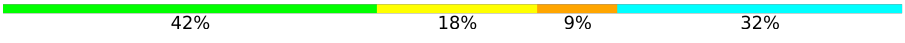
Chain B:

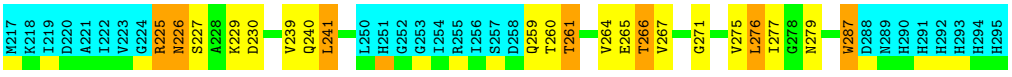




• Molecule 1: Small s protein

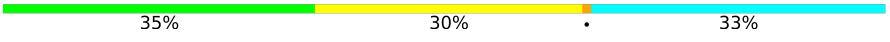
Chain C:





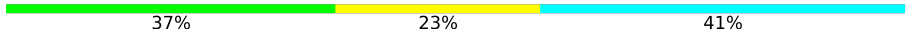
• Molecule 1: Small s protein

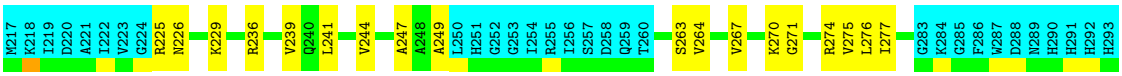
Chain D:



• Molecule 1: Small s protein

Chain E:

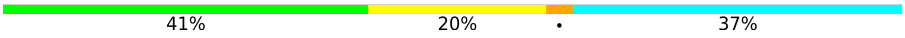




4.2.2 Score per residue for model 2

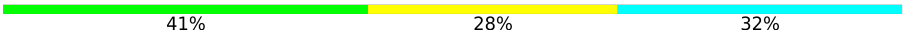
• Molecule 1: Small s protein

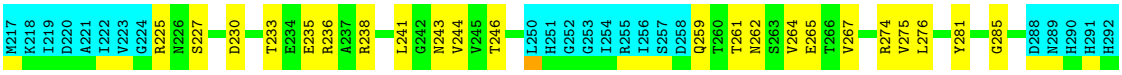
Chain A:



• Molecule 1: Small s protein

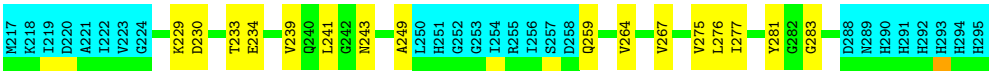
Chain B:





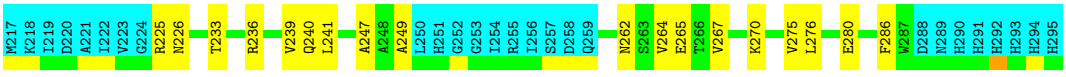
• Molecule 1: Small s protein

Chain C:



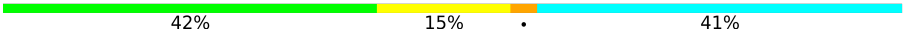
• Molecule 1: Small s protein

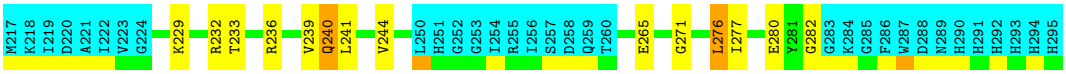
Chain D:



• Molecule 1: Small s protein

Chain E:

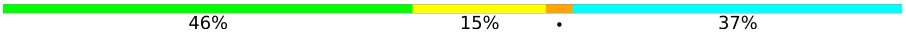


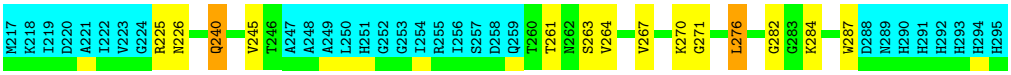


4.2.3 Score per residue for model 3

• Molecule 1: Small s protein

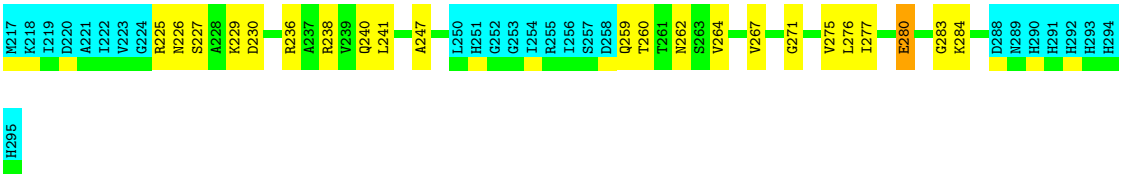
Chain A:





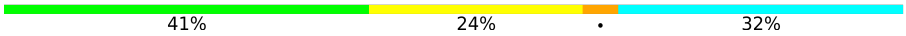
• Molecule 1: Small s protein

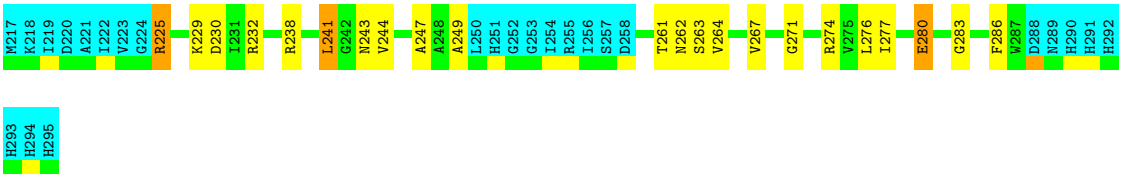
Chain B:



• Molecule 1: Small s protein

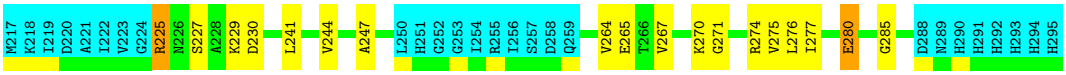
Chain C:





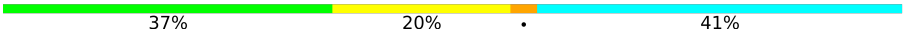
• Molecule 1: Small s protein

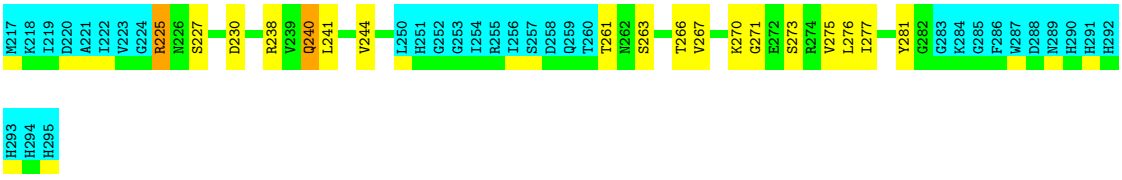
Chain D:



• Molecule 1: Small s protein

Chain E:

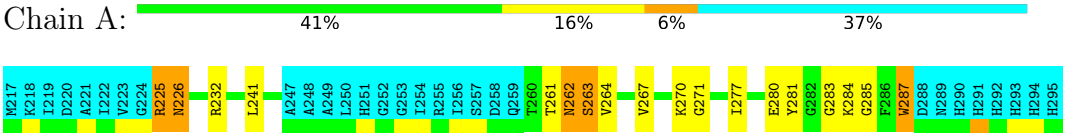




4.2.4 Score per residue for model 4

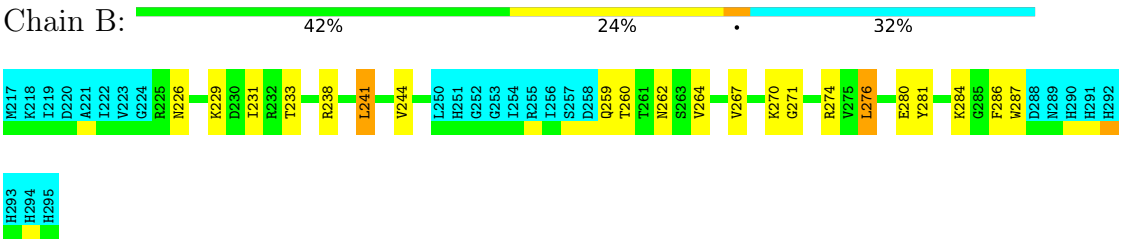
• Molecule 1: Small s protein

Chain A:



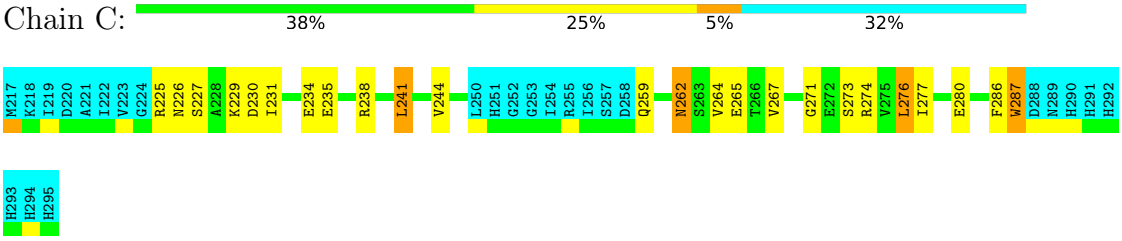
• Molecule 1: Small s protein

Chain B:



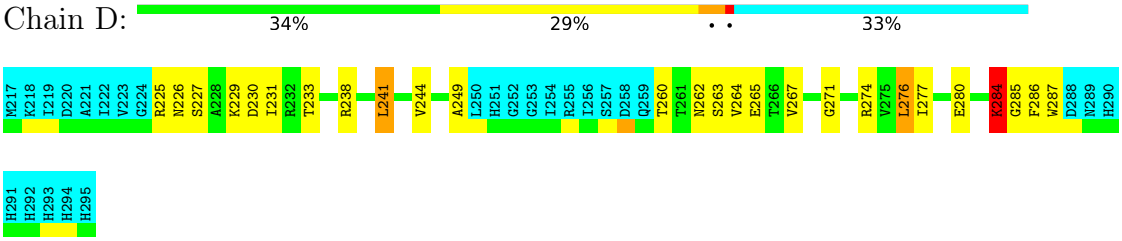
• Molecule 1: Small s protein

Chain C:



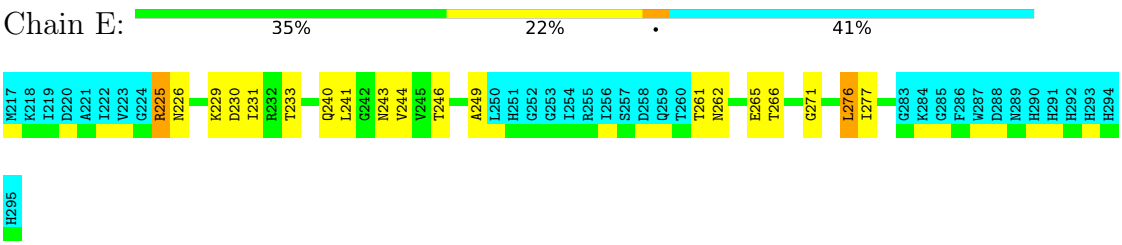
• Molecule 1: Small s protein

Chain D:



• Molecule 1: Small s protein

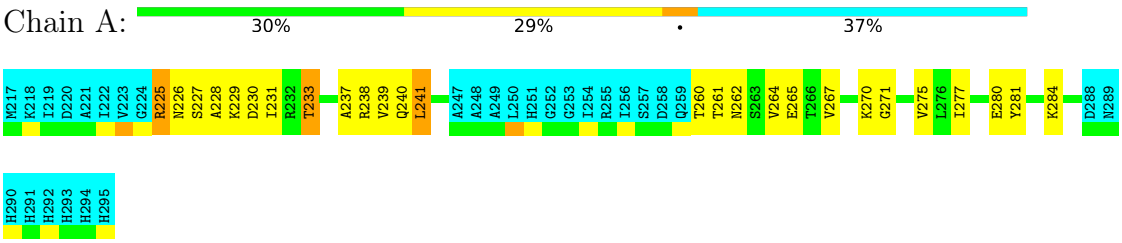
Chain E:



4.2.5 Score per residue for model 5

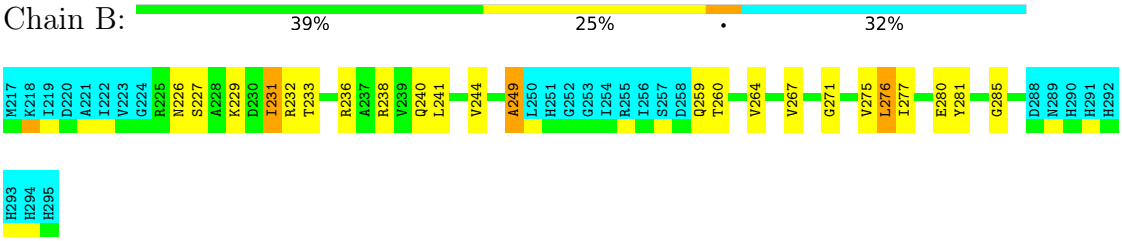
• Molecule 1: Small s protein

Chain A:



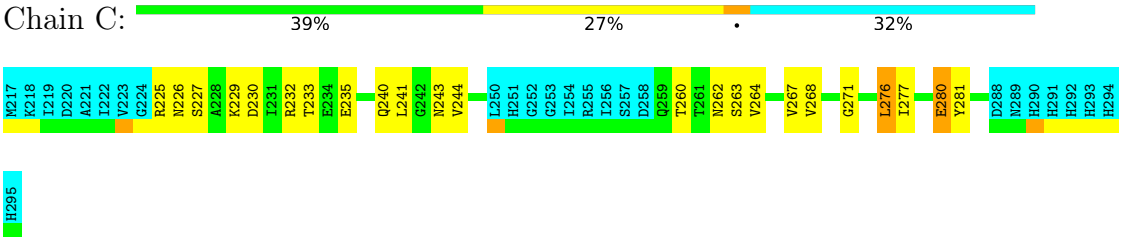
• Molecule 1: Small s protein

Chain B:



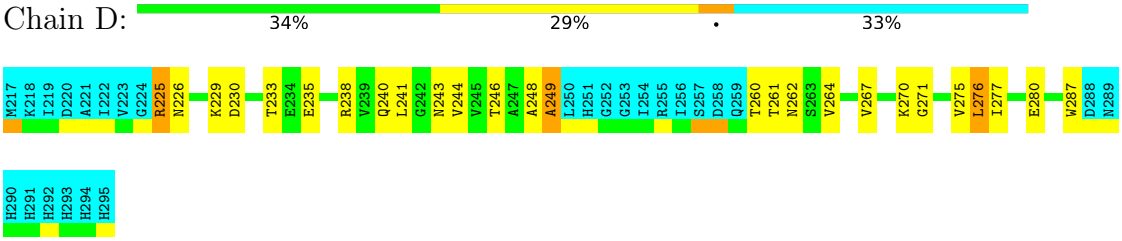
• Molecule 1: Small s protein

Chain C:



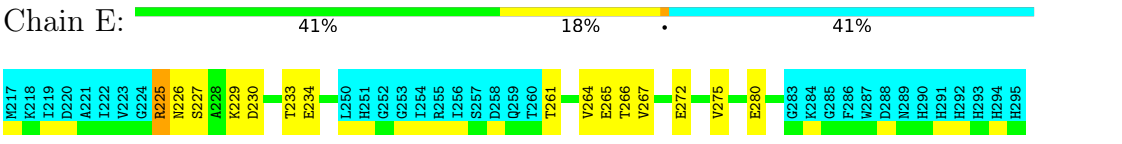
• Molecule 1: Small s protein

Chain D:



• Molecule 1: Small s protein

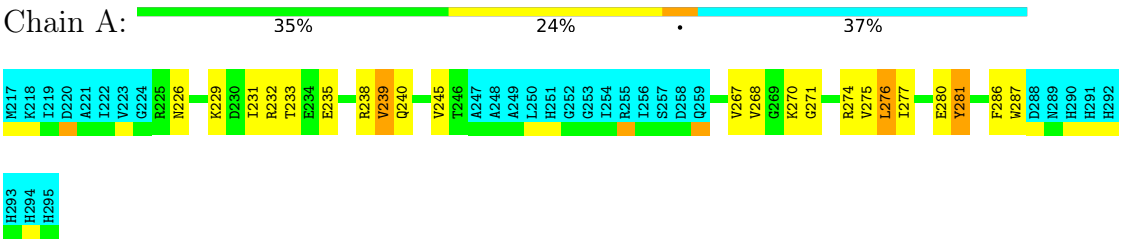
Chain E:



4.2.6 Score per residue for model 6

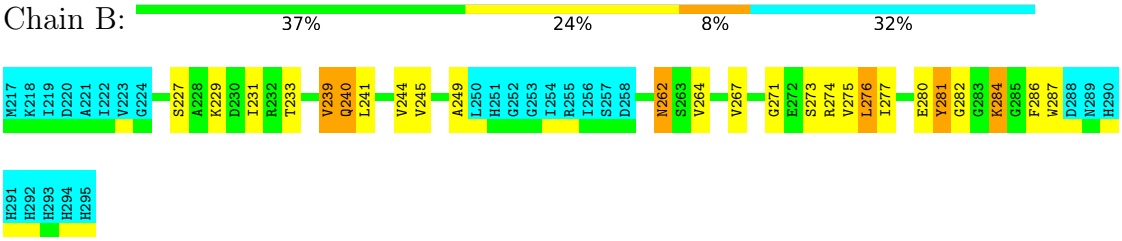
• Molecule 1: Small s protein

Chain A:



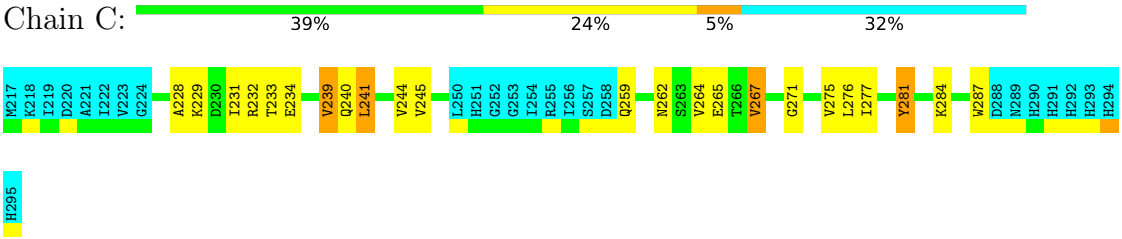
• Molecule 1: Small s protein

Chain B:



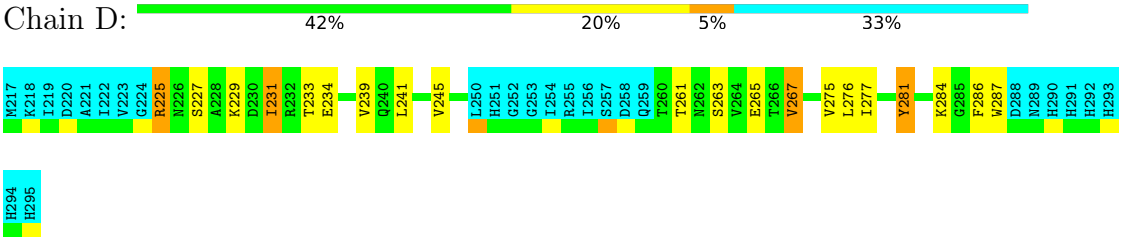
• Molecule 1: Small s protein

Chain C:



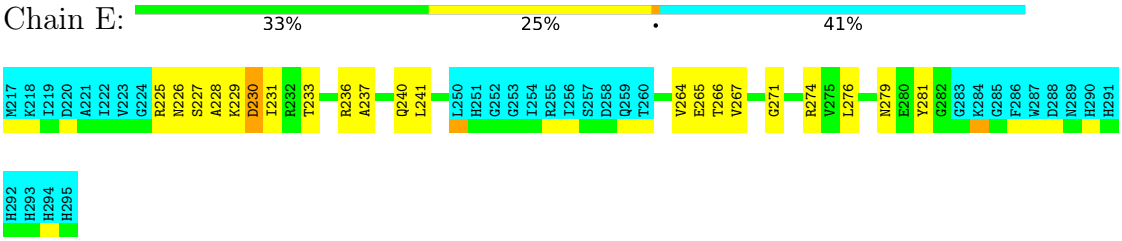
• Molecule 1: Small s protein

Chain D:



• Molecule 1: Small s protein

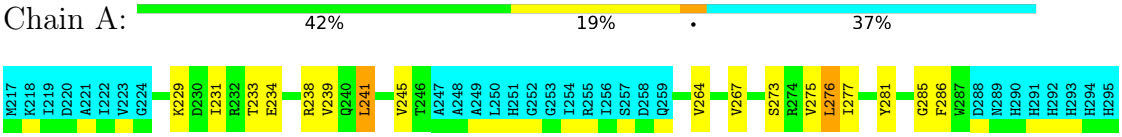
Chain E:



4.2.7 Score per residue for model 7

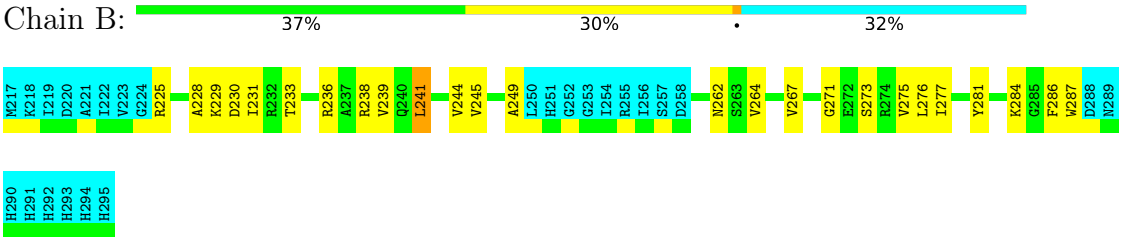
• Molecule 1: Small s protein

Chain A:



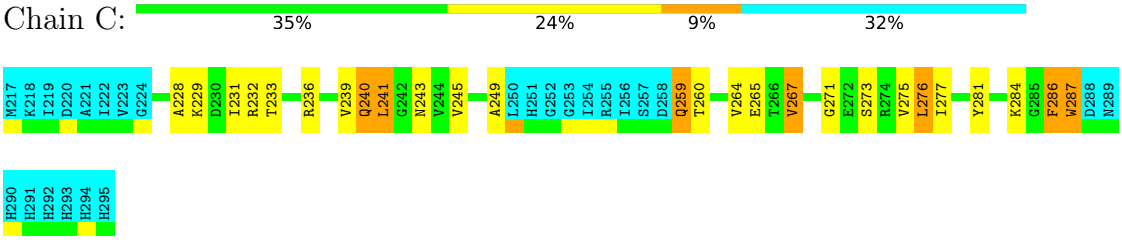
• Molecule 1: Small s protein

Chain B:



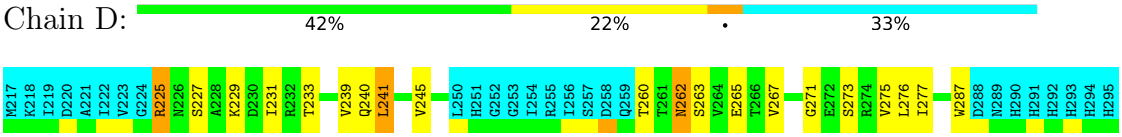
• Molecule 1: Small s protein

Chain C:



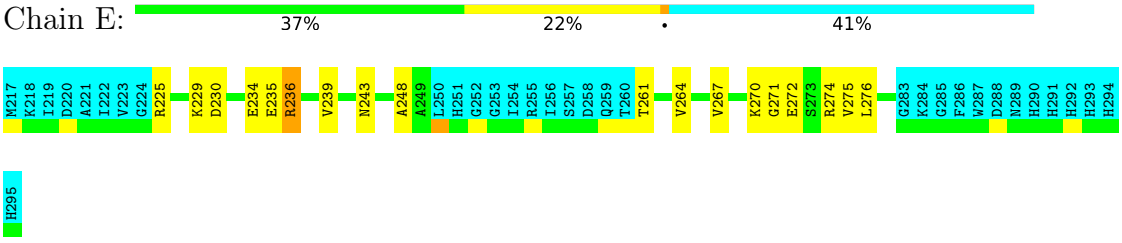
• Molecule 1: Small s protein

Chain D:



• Molecule 1: Small s protein

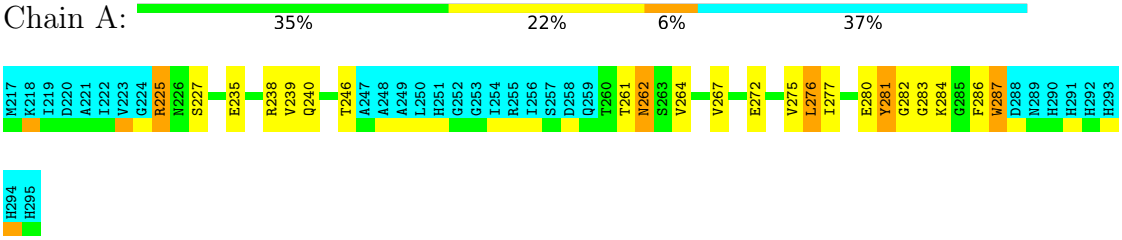
Chain E:



4.2.8 Score per residue for model 8

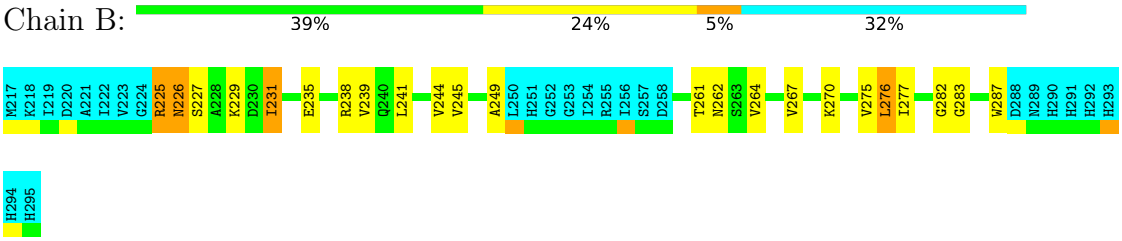
• Molecule 1: Small s protein

Chain A:



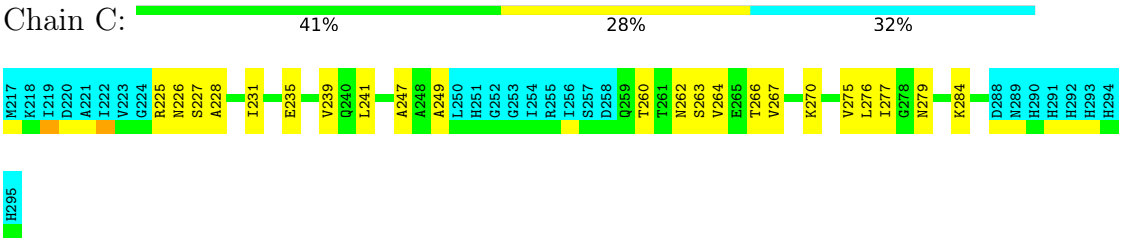
• Molecule 1: Small s protein

Chain B:



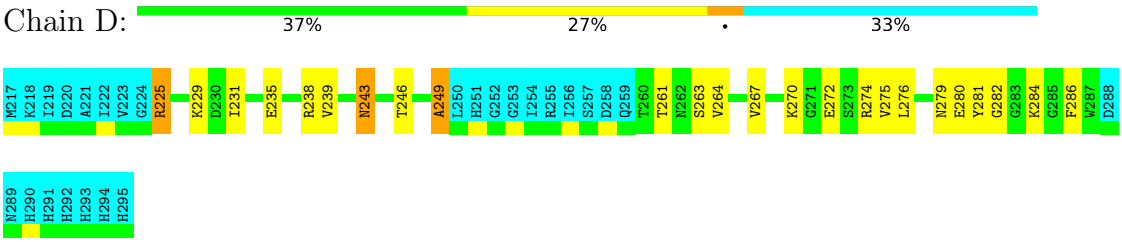
• Molecule 1: Small s protein

Chain C:



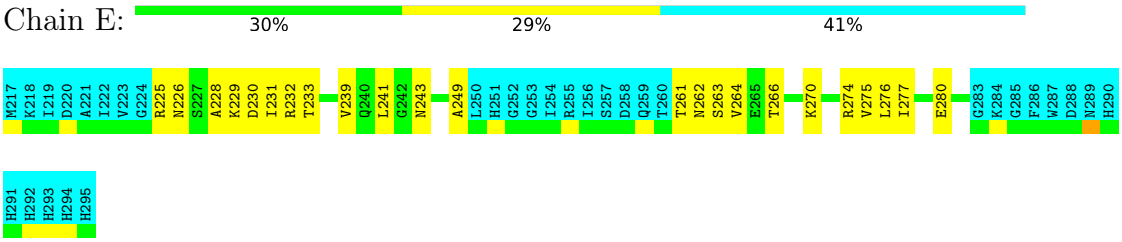
• Molecule 1: Small s protein

Chain D:



• Molecule 1: Small s protein

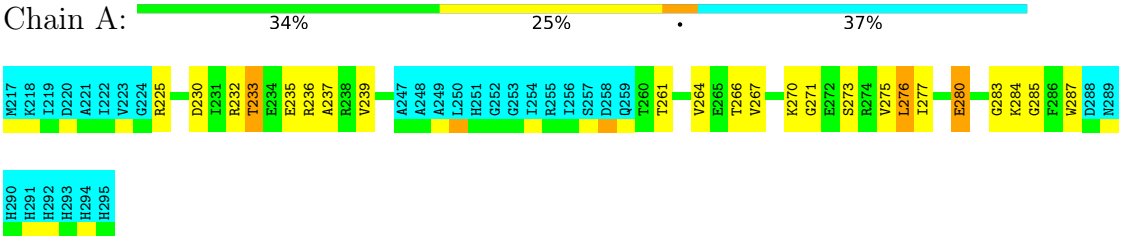
Chain E:



4.2.9 Score per residue for model 9

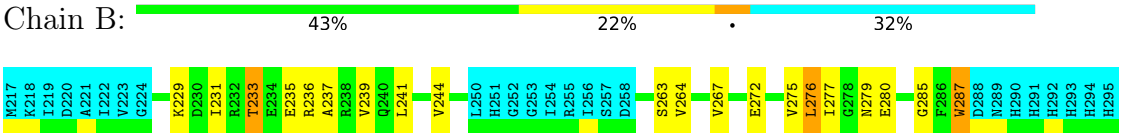
• Molecule 1: Small s protein

Chain A:



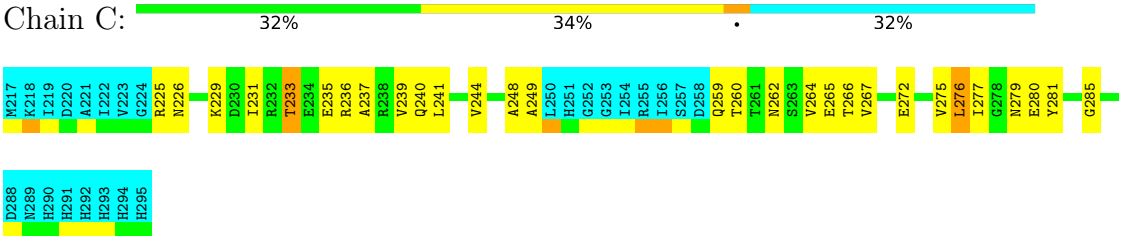
• Molecule 1: Small s protein

Chain B:



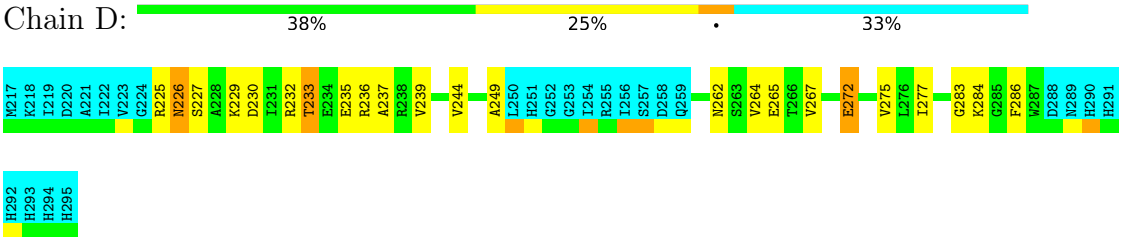
• Molecule 1: Small s protein

Chain C:



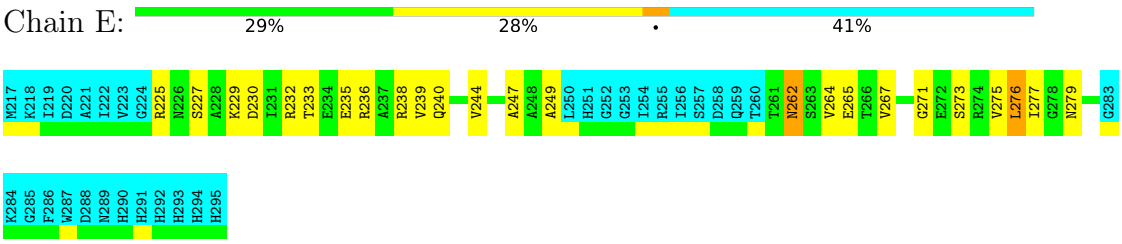
• Molecule 1: Small s protein

Chain D:



• Molecule 1: Small s protein

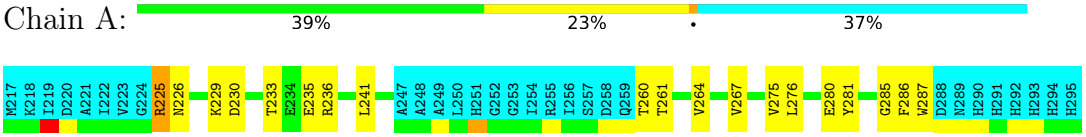
Chain E:



4.2.10 Score per residue for model 10

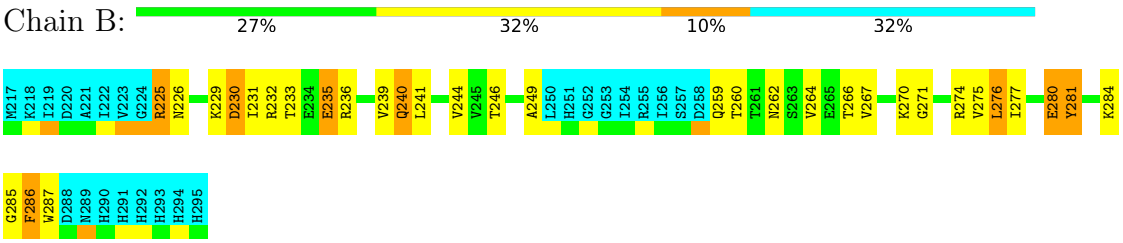
• Molecule 1: Small s protein

Chain A:



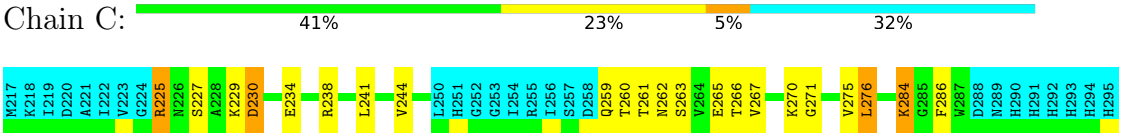
• Molecule 1: Small s protein

Chain B:



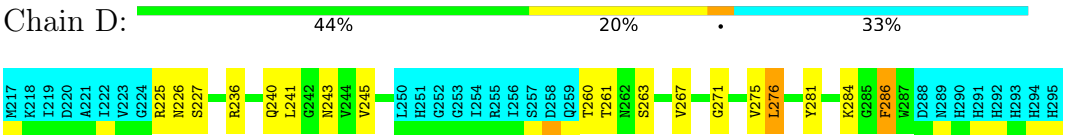
• Molecule 1: Small s protein

Chain C:



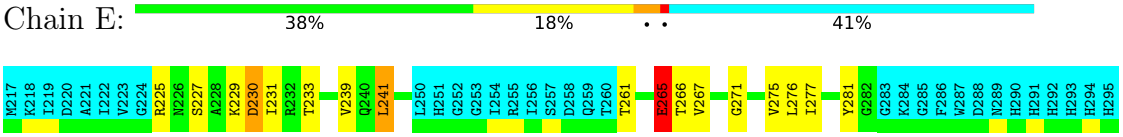
• Molecule 1: Small s protein

Chain D:



• Molecule 1: Small s protein

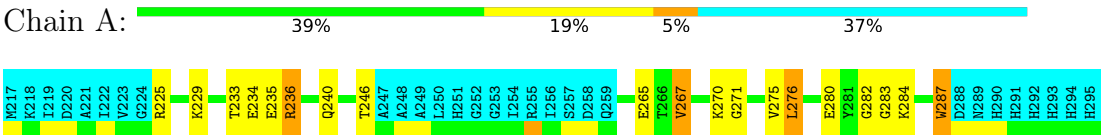
Chain E:



4.2.11 Score per residue for model 11

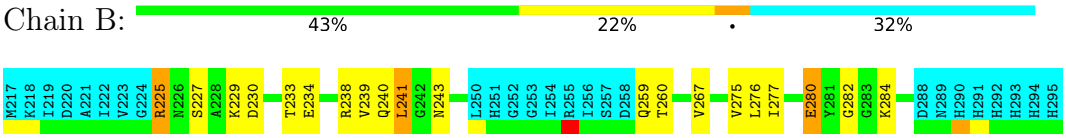
• Molecule 1: Small s protein

Chain A:



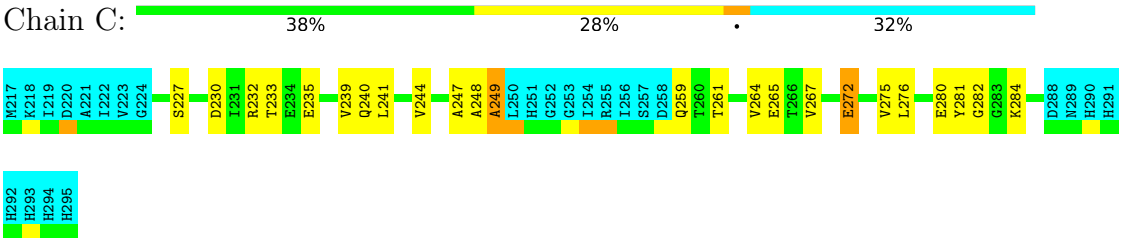
• Molecule 1: Small s protein

Chain B:



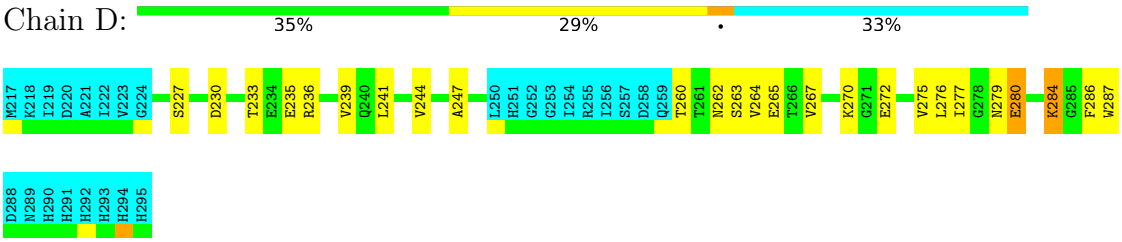
• Molecule 1: Small s protein

Chain C:



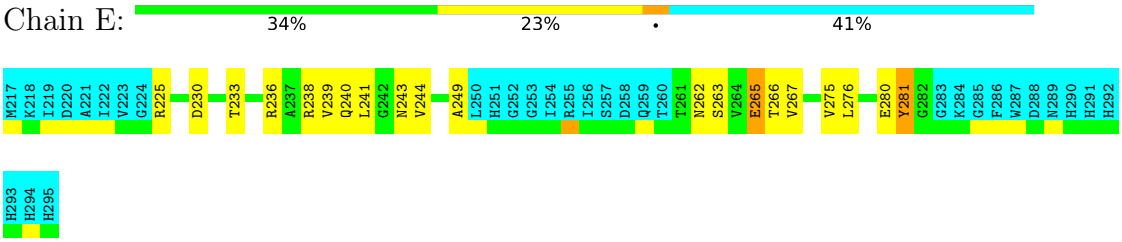
• Molecule 1: Small s protein

Chain D:



• Molecule 1: Small s protein

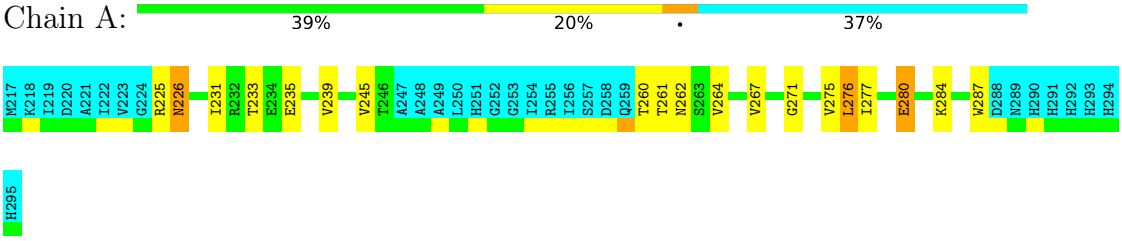
Chain E:



4.2.12 Score per residue for model 12

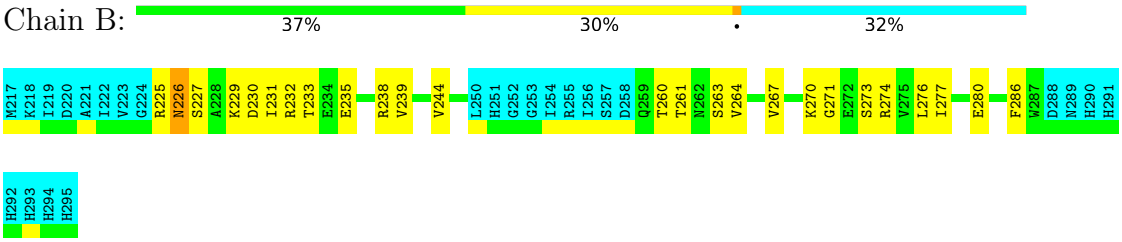
• Molecule 1: Small s protein

Chain A:



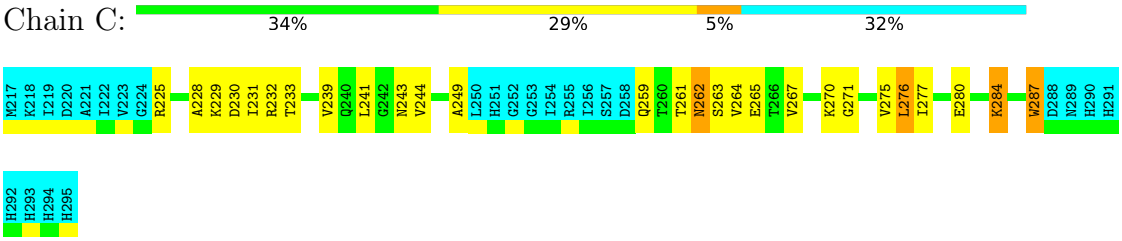
• Molecule 1: Small s protein

Chain B:



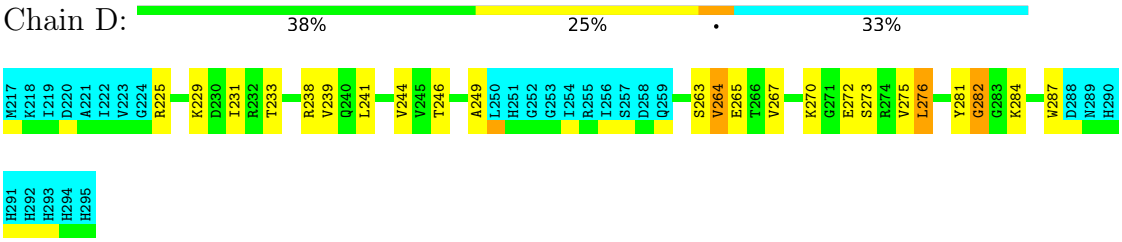
• Molecule 1: Small s protein

Chain C:



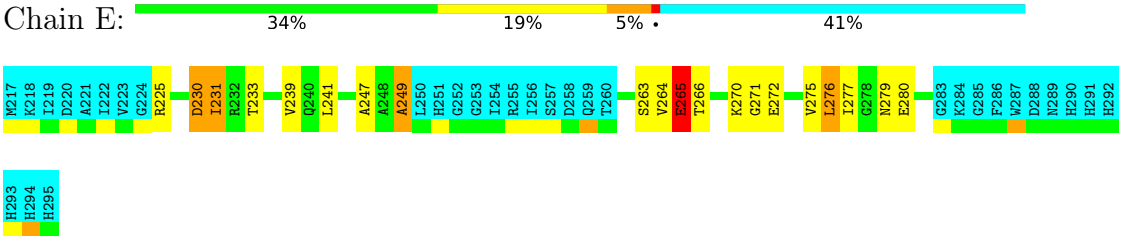
• Molecule 1: Small s protein

Chain D:



• Molecule 1: Small s protein

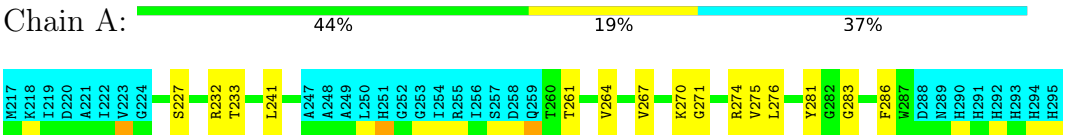
Chain E:



4.2.13 Score per residue for model 13

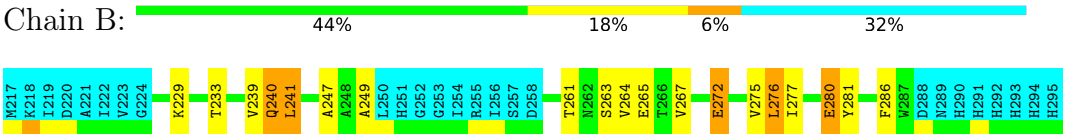
• Molecule 1: Small s protein

Chain A:



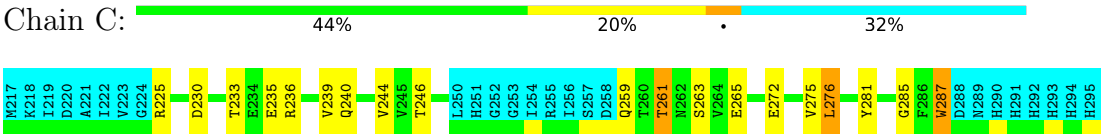
• Molecule 1: Small s protein

Chain B:



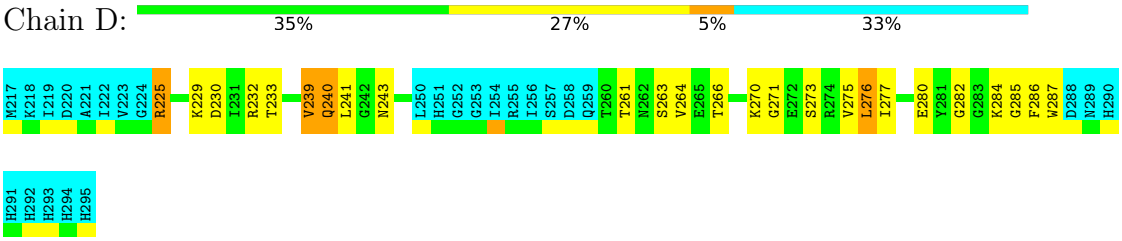
• Molecule 1: Small s protein

Chain C:



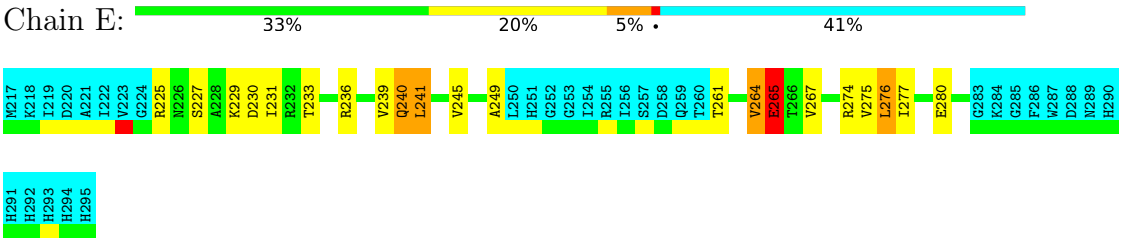
• Molecule 1: Small s protein

Chain D:



• Molecule 1: Small s protein

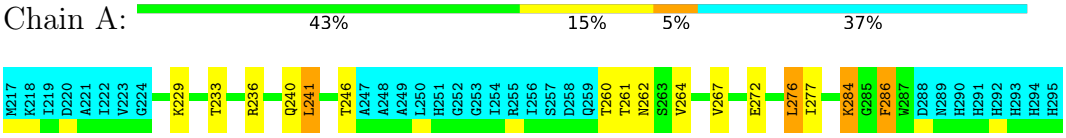
Chain E:



4.2.14 Score per residue for model 14

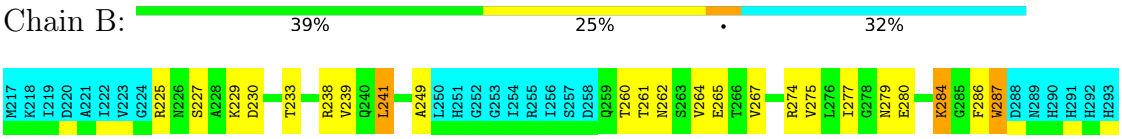
• Molecule 1: Small s protein

Chain A:



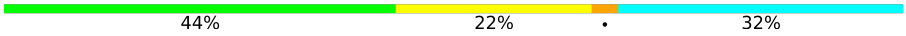
• Molecule 1: Small s protein

Chain B:



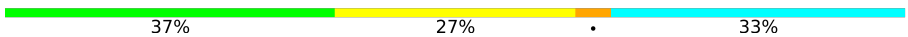
• Molecule 1: Small s protein

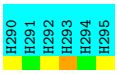
Chain C:



• Molecule 1: Small s protein

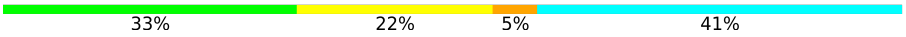
Chain D:





• Molecule 1: Small s protein

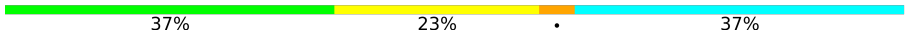
Chain E:

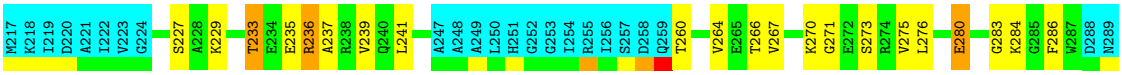


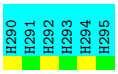
4.2.15 Score per residue for model 15

• Molecule 1: Small s protein

Chain A:

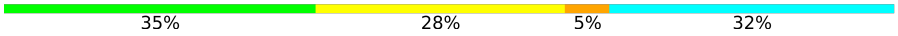


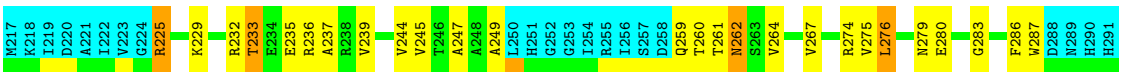




• Molecule 1: Small s protein

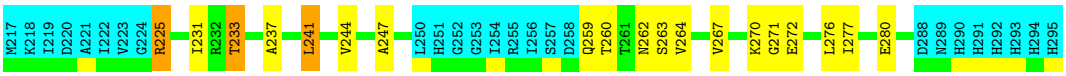
Chain B:





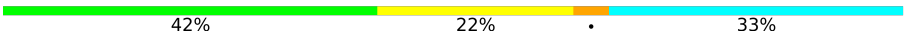
• Molecule 1: Small s protein

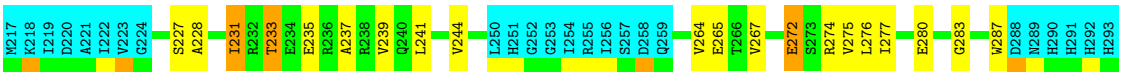
Chain C:



• Molecule 1: Small s protein

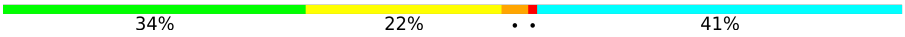
Chain D:

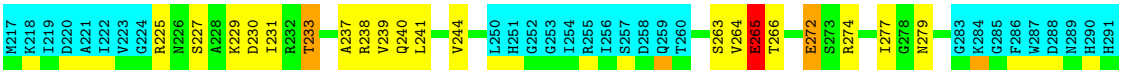




• Molecule 1: Small s protein

Chain E:

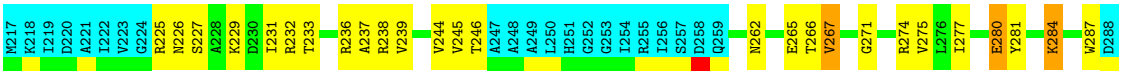


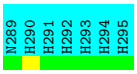


4.2.16 Score per residue for model 16

• Molecule 1: Small s protein

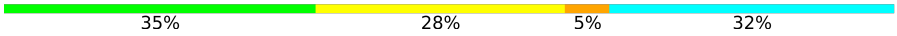
Chain A:

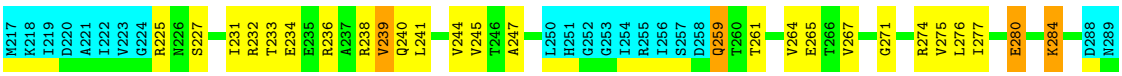


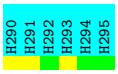


• Molecule 1: Small s protein

Chain B:

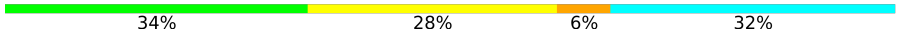


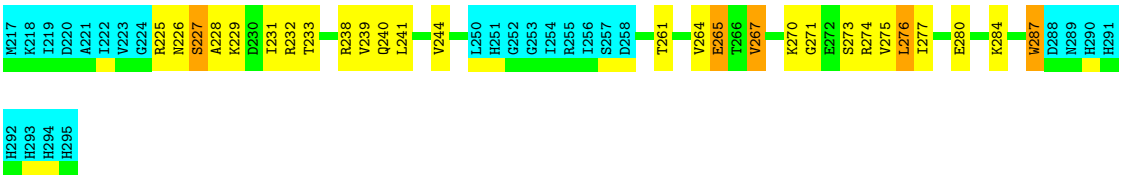




• Molecule 1: Small s protein

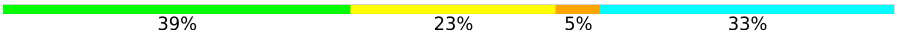
Chain C:

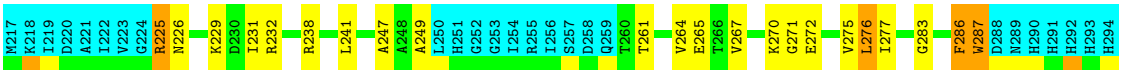




• Molecule 1: Small s protein

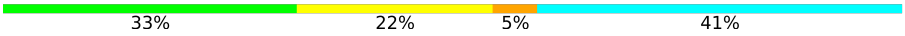
Chain D:





• Molecule 1: Small s protein

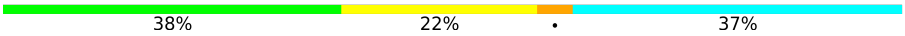
Chain E:

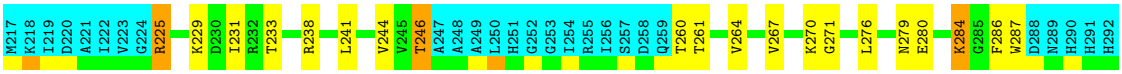


4.2.17 Score per residue for model 17

• Molecule 1: Small s protein

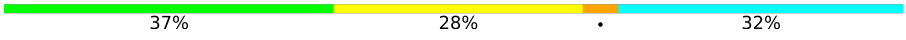
Chain A:

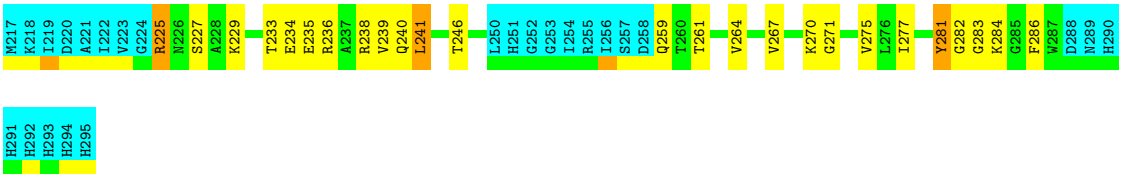




• Molecule 1: Small s protein

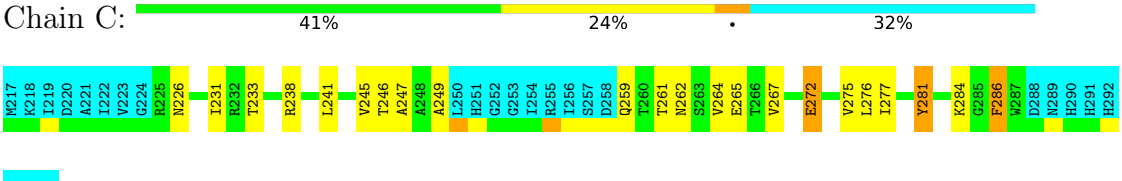
Chain B:





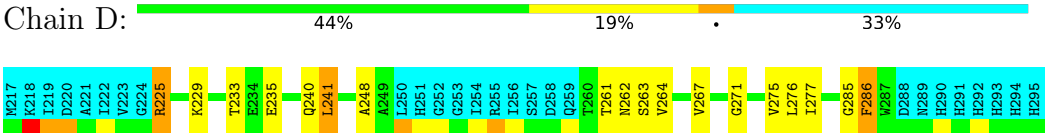
• Molecule 1: Small s protein

Chain C:



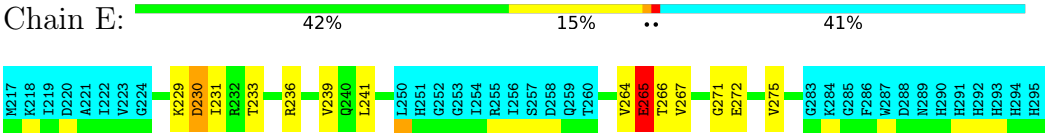
• Molecule 1: Small s protein

Chain D:



• Molecule 1: Small s protein

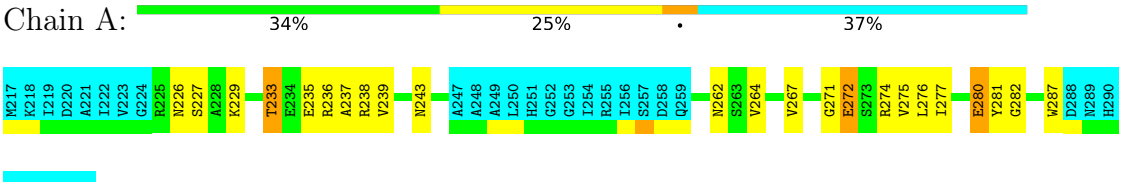
Chain E:



4.2.18 Score per residue for model 18

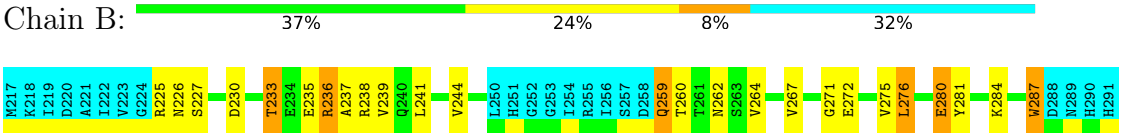
• Molecule 1: Small s protein

Chain A:



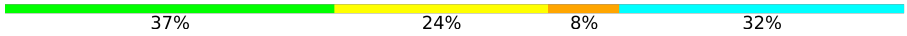
• Molecule 1: Small s protein

Chain B:



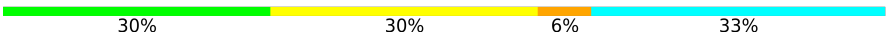
• Molecule 1: Small s protein

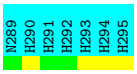
Chain C:



• Molecule 1: Small s protein

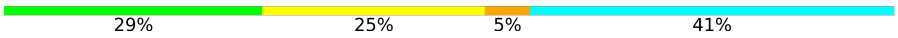
Chain D:

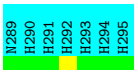




• Molecule 1: Small s protein

Chain E:

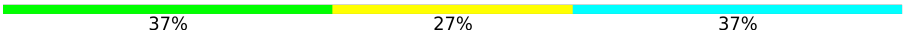




4.2.19 Score per residue for model 19 (medoid)

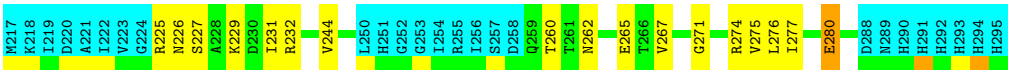
• Molecule 1: Small s protein

Chain A:



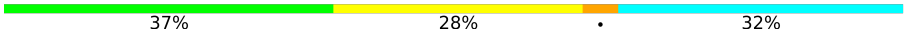
• Molecule 1: Small s protein

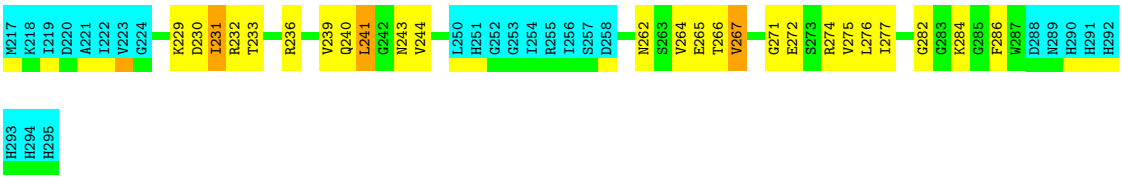
Chain B:



• Molecule 1: Small s protein

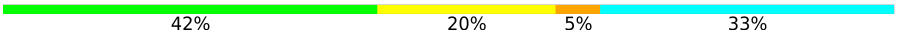
Chain C:

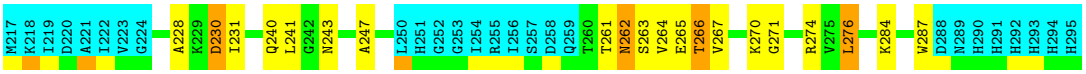




• Molecule 1: Small s protein

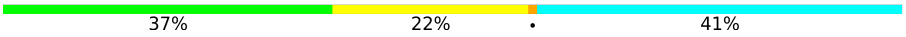
Chain D:

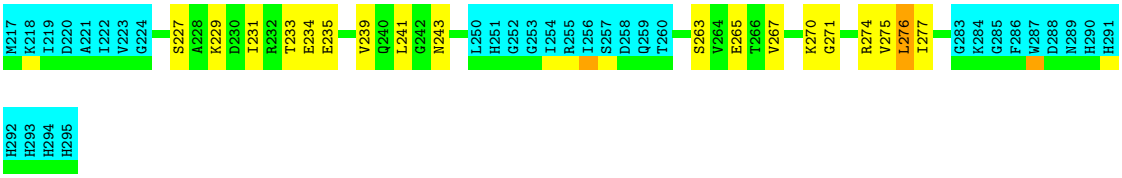




• Molecule 1: Small s protein

Chain E:

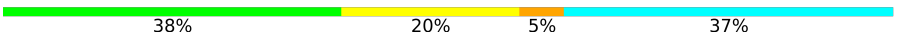


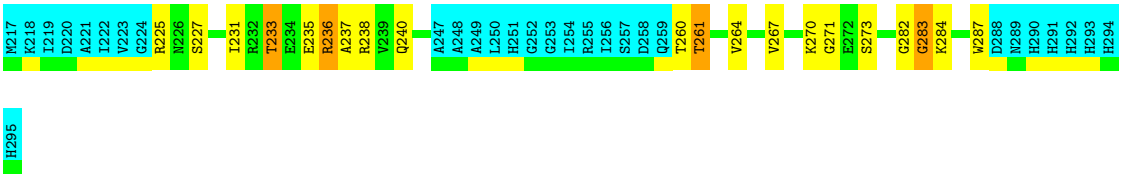


4.2.20 Score per residue for model 20

• Molecule 1: Small s protein

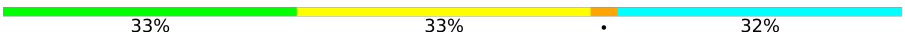
Chain A:

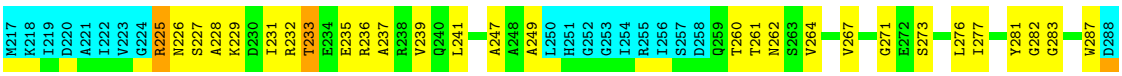


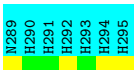


• Molecule 1: Small s protein

Chain B:

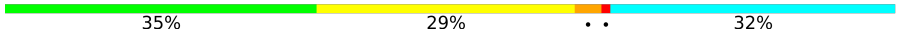


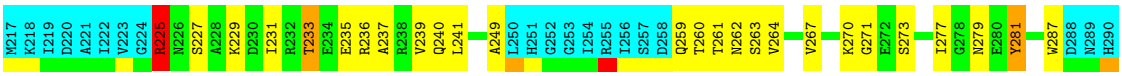




• Molecule 1: Small s protein

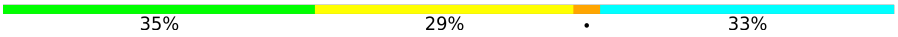
Chain C:

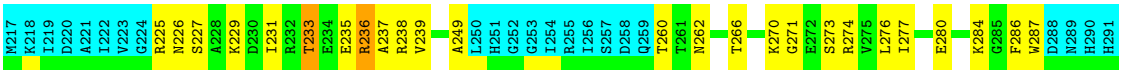




• Molecule 1: Small s protein

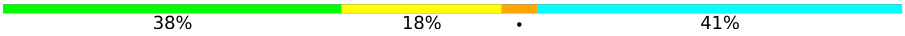
Chain D:





• Molecule 1: Small s protein

Chain E:



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: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	refinement	2.1

No chemical shift data was provided.

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	385	386	386	9±4
1	B	409	409	409	14±4
1	C	409	409	409	14±4
1	D	400	401	401	13±3
1	E	351	356	356	9±3
All	All	39080	39220	39220	908

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:264:VAL:HG21	1:E:277:ILE:HD12	0.90	1.43	12	2
1:A:267:VAL:HG11	1:A:275:VAL:HG21	0.89	1.45	18	2
1:C:277:ILE:HD13	1:D:241:LEU:HD23	0.88	1.46	1	1
1:C:241:LEU:HD12	1:C:277:ILE:HD13	0.88	1.46	3	3
1:D:267:VAL:HG11	1:D:275:VAL:HG11	0.87	1.46	6	3
1:B:277:ILE:HD13	1:C:241:LEU:HD23	0.87	1.43	1	1
1:E:267:VAL:HG11	1:E:275:VAL:HG21	0.84	1.45	17	7
1:B:264:VAL:HG21	1:B:277:ILE:HD12	0.82	1.49	9	1
1:D:241:LEU:HD12	1:D:277:ILE:HD12	0.82	1.49	17	2
1:E:264:VAL:HG21	1:E:277:ILE:HD13	0.79	1.54	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:267:VAL:HG13	1:B:231:ILE:HD11	0.78	1.54	16	1
1:E:241:LEU:HD12	1:E:277:ILE:HD12	0.76	1.55	13	3
1:E:231:ILE:HD12	1:E:239:VAL:HG11	0.75	1.58	20	1
1:B:267:VAL:HG11	1:B:275:VAL:HG21	0.73	1.59	18	2
1:C:267:VAL:HG22	1:D:231:ILE:HD11	0.71	1.63	12	2
1:C:267:VAL:HG11	1:C:275:VAL:HG11	0.71	1.62	6	1
1:C:241:LEU:HD12	1:C:277:ILE:HD12	0.70	1.62	7	1
1:A:241:LEU:HD23	1:A:277:ILE:HD13	0.69	1.65	7	2
1:A:267:VAL:HG22	1:B:231:ILE:HD11	0.68	1.65	4	4
1:A:228:ALA:HB1	1:A:231:ILE:HD11	0.67	1.63	1	1
1:C:276:LEU:HD12	1:C:287:TRP:CE2	0.67	2.24	16	1
1:C:286:PHE:CE1	1:D:276:LEU:HD11	0.67	2.24	7	1
1:C:231:ILE:HG22	1:C:267:VAL:HG22	0.67	1.67	7	1
1:C:264:VAL:HG11	1:C:267:VAL:HG23	0.67	1.67	9	1
1:C:264:VAL:HG21	1:C:277:ILE:HD12	0.66	1.66	9	1
1:D:264:VAL:HG23	1:E:241:LEU:HD22	0.66	1.66	12	1
1:D:264:VAL:HA	1:E:228:ALA:HB3	0.66	1.65	14	1
1:D:264:VAL:HG22	1:E:231:ILE:HD11	0.66	1.67	12	1
1:A:264:VAL:HG23	1:B:228:ALA:HB3	0.65	1.67	7	1
1:A:280:GLU:CG	1:B:244:VAL:HG12	0.65	2.21	16	5
1:B:264:VAL:HG21	1:C:231:ILE:HD11	0.65	1.67	7	4
1:A:246:THR:HG22	1:A:281:TYR:O	0.65	1.92	16	1
1:E:241:LEU:HD12	1:E:277:ILE:HB	0.65	1.68	8	1
1:A:264:VAL:HG21	1:B:231:ILE:CD1	0.65	2.22	7	4
1:E:225:ARG:O	1:E:261:THR:HG23	0.64	1.92	3	1
1:D:280:GLU:CG	1:E:244:VAL:HG22	0.64	2.22	11	2
1:A:262:ASN:OD1	1:A:277:ILE:HG23	0.64	1.92	19	2
1:D:245:VAL:HG12	1:D:281:TYR:HB2	0.64	1.67	6	1
1:B:233:THR:OG1	1:B:237:ALA:HB3	0.64	1.92	15	3
1:A:228:ALA:CB	1:A:231:ILE:HD11	0.64	2.23	1	1
1:D:280:GLU:CG	1:E:244:VAL:HG13	0.64	2.23	18	2
1:C:286:PHE:CZ	1:D:276:LEU:HD11	0.64	2.27	7	1
1:B:241:LEU:HD23	1:B:277:ILE:HD13	0.64	1.68	13	2
1:B:264:VAL:HG11	1:B:267:VAL:HG23	0.64	1.68	9	1
1:D:241:LEU:HD13	1:D:277:ILE:HB	0.64	1.68	15	4
1:A:226:ASN:OD1	1:A:277:ILE:HG22	0.64	1.93	6	4
1:B:264:VAL:HG21	1:B:267:VAL:CG1	0.64	2.23	16	2
1:D:267:VAL:HG22	1:E:231:ILE:HD12	0.64	1.67	12	1
1:D:264:VAL:HG21	1:E:231:ILE:CD1	0.63	2.22	4	1
1:E:267:VAL:CG1	1:E:275:VAL:HG21	0.63	2.22	13	7
1:C:280:GLU:CG	1:D:244:VAL:HG23	0.63	2.24	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:286:PHE:CZ	1:B:244:VAL:HG11	0.63	2.29	15	1
1:D:286:PHE:CE1	1:E:244:VAL:HG11	0.63	2.28	16	1
1:E:241:LEU:CD1	1:E:277:ILE:HD12	0.63	2.23	13	2
1:C:262:ASN:OD1	1:C:277:ILE:HG23	0.63	1.93	19	3
1:A:233:THR:OG1	1:A:237:ALA:HB3	0.63	1.94	15	6
1:C:264:VAL:HG23	1:D:231:ILE:HD11	0.63	1.71	15	2
1:C:283:GLY:N	1:D:247:ALA:HB2	0.63	2.08	3	3
1:E:241:LEU:HD13	1:E:277:ILE:HB	0.63	1.71	2	5
1:B:280:GLU:CG	1:C:244:VAL:HG13	0.62	2.25	18	2
1:D:262:ASN:OD1	1:D:277:ILE:HG22	0.62	1.94	18	1
1:B:267:VAL:CG1	1:B:275:VAL:HG21	0.62	2.24	18	4
1:C:241:LEU:HD12	1:C:277:ILE:CG1	0.62	2.25	1	1
1:A:277:ILE:CD1	1:B:241:LEU:HD13	0.62	2.23	18	5
1:C:233:THR:OG1	1:C:237:ALA:HB3	0.62	1.95	20	4
1:D:276:LEU:HD12	1:D:287:TRP:CD1	0.62	2.29	13	1
1:C:246:THR:HG22	1:C:281:TYR:CD2	0.62	2.30	13	1
1:B:276:LEU:HD22	1:B:287:TRP:CE3	0.62	2.29	4	1
1:B:262:ASN:OD1	1:B:277:ILE:HG23	0.62	1.95	19	1
1:D:286:PHE:CE1	1:E:244:VAL:HG21	0.62	2.30	1	1
1:D:275:VAL:HG13	1:E:239:VAL:HG23	0.62	1.70	13	4
1:A:241:LEU:CD2	1:A:277:ILE:HD13	0.62	2.24	7	2
1:B:225:ARG:O	1:B:261:THR:HG23	0.62	1.94	8	2
1:A:280:GLU:HG3	1:B:244:VAL:HG23	0.62	1.71	5	2
1:C:231:ILE:HG22	1:C:267:VAL:CG2	0.62	2.25	7	5
1:C:280:GLU:CG	1:D:244:VAL:HG22	0.62	2.25	5	4
1:D:275:VAL:O	1:D:276:LEU:HD23	0.62	1.93	6	1
1:D:267:VAL:HG11	1:D:275:VAL:HG21	0.61	1.72	18	4
1:D:264:VAL:HG21	1:D:267:VAL:HG23	0.61	1.71	19	1
1:A:280:GLU:CG	1:B:244:VAL:HG22	0.61	2.25	18	1
1:A:280:GLU:HG2	1:B:244:VAL:HG22	0.61	1.71	18	1
1:B:225:ARG:CB	1:B:261:THR:HG23	0.61	2.26	2	2
1:D:260:THR:HG21	1:E:243:ASN:CG	0.61	2.16	4	1
1:E:231:ILE:HG21	1:E:239:VAL:HG21	0.61	1.72	19	2
1:C:240:GLN:C	1:C:241:LEU:HD13	0.61	2.16	1	3
1:A:276:LEU:HD12	1:A:287:TRP:CE2	0.61	2.31	8	2
1:C:241:LEU:HD13	1:C:277:ILE:HB	0.61	1.73	2	4
1:C:264:VAL:HG21	1:D:231:ILE:HD11	0.61	1.72	16	3
1:C:280:GLU:HG3	1:D:244:VAL:HG13	0.61	1.72	3	1
1:A:245:VAL:HG12	1:A:281:TYR:CB	0.61	2.25	6	1
1:D:245:VAL:HG12	1:D:281:TYR:CB	0.61	2.26	6	1
1:D:280:GLU:HG3	1:E:244:VAL:HG23	0.60	1.72	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:264:VAL:HG11	1:C:267:VAL:CG2	0.60	2.27	9	1
1:C:281:TYR:CE1	1:D:249:ALA:HB2	0.60	2.31	5	1
1:A:267:VAL:HG11	1:A:275:VAL:HG11	0.60	1.72	11	1
1:D:280:GLU:OE1	1:E:244:VAL:HG13	0.60	1.96	11	1
1:D:267:VAL:CG1	1:D:275:VAL:HG21	0.60	2.26	17	7
1:C:267:VAL:CG1	1:C:275:VAL:HG21	0.60	2.26	17	5
1:D:241:LEU:CD2	1:D:277:ILE:HD13	0.60	2.27	15	1
1:B:245:VAL:HG12	1:B:281:TYR:CB	0.60	2.27	6	1
1:D:225:ARG:O	1:D:261:THR:HG23	0.60	1.97	17	2
1:A:286:PHE:CE2	1:B:244:VAL:HG11	0.60	2.31	15	1
1:C:239:VAL:HG12	1:C:275:VAL:HB	0.60	1.74	9	6
1:C:260:THR:HG21	1:C:279:ASN:HB3	0.60	1.71	9	1
1:B:267:VAL:HG22	1:C:231:ILE:HD11	0.60	1.73	12	3
1:B:240:GLN:C	1:B:241:LEU:HD13	0.60	2.16	1	1
1:E:231:ILE:HG23	1:E:267:VAL:CG2	0.60	2.27	6	1
1:B:226:ASN:OD1	1:B:277:ILE:HG22	0.60	1.96	19	2
1:D:241:LEU:HD12	1:D:277:ILE:CG1	0.60	2.27	1	2
1:A:228:ALA:HB2	1:A:241:LEU:HD21	0.59	1.73	5	1
1:D:264:VAL:HG21	1:D:277:ILE:HD12	0.59	1.72	9	1
1:C:249:ALA:HB2	1:C:281:TYR:CD1	0.59	2.32	2	1
1:D:239:VAL:HG12	1:D:275:VAL:HB	0.59	1.73	9	4
1:C:267:VAL:HG11	1:C:275:VAL:HG21	0.59	1.74	18	4
1:D:280:GLU:HG2	1:E:244:VAL:HG13	0.59	1.74	18	1
1:B:241:LEU:HD12	1:B:277:ILE:CG1	0.59	2.27	1	1
1:A:267:VAL:HG13	1:B:231:ILE:CD1	0.59	2.26	16	1
1:A:267:VAL:CG1	1:A:275:VAL:HG21	0.59	2.26	18	1
1:B:264:VAL:CG1	1:B:267:VAL:HG23	0.59	2.27	9	1
1:A:231:ILE:HG22	1:A:267:VAL:CG1	0.59	2.28	19	1
1:C:241:LEU:CD1	1:C:277:ILE:HD13	0.59	2.26	3	2
1:A:264:VAL:HG21	1:A:277:ILE:HD12	0.59	1.75	9	1
1:E:239:VAL:HG12	1:E:275:VAL:HB	0.59	1.75	9	4
1:E:241:LEU:HD22	1:E:277:ILE:HB	0.59	1.74	10	1
1:C:245:VAL:HG12	1:C:281:TYR:HB2	0.59	1.74	6	1
1:B:277:ILE:CD1	1:C:241:LEU:HD13	0.59	2.28	16	2
1:B:226:ASN:HB3	1:B:277:ILE:HG22	0.58	1.75	8	3
1:C:260:THR:HG21	1:D:243:ASN:OD1	0.58	1.97	5	2
1:A:276:LEU:HD12	1:A:287:TRP:CD2	0.58	2.32	9	1
1:A:225:ARG:CB	1:A:261:THR:HG23	0.58	2.29	4	1
1:A:231:ILE:HD12	1:A:239:VAL:HG21	0.58	1.74	5	1
1:B:239:VAL:HG12	1:B:275:VAL:HB	0.58	1.75	11	7
1:B:233:THR:HG21	1:B:239:VAL:HG13	0.58	1.74	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:280:GLU:HG3	1:B:244:VAL:HG12	0.58	1.75	16	5
1:D:280:GLU:CG	1:E:244:VAL:HG12	0.58	2.27	2	1
1:E:231:ILE:HG23	1:E:267:VAL:CG1	0.58	2.28	19	2
1:E:231:ILE:CG2	1:E:239:VAL:HG11	0.58	2.29	15	2
1:C:276:LEU:HD13	1:C:287:TRP:CE3	0.58	2.33	4	1
1:B:233:THR:CB	1:B:237:ALA:HB3	0.58	2.29	20	4
1:C:276:LEU:HD12	1:C:287:TRP:CD1	0.58	2.34	13	1
1:D:240:GLN:C	1:D:241:LEU:HD13	0.58	2.18	1	3
1:B:264:VAL:HG21	1:C:231:ILE:CD1	0.58	2.29	12	3
1:D:240:GLN:HB3	1:D:276:LEU:HD22	0.58	1.76	5	2
1:B:262:ASN:HB3	1:C:241:LEU:HD23	0.58	1.74	15	1
1:B:231:ILE:HG22	1:B:267:VAL:CG1	0.58	2.28	19	1
1:C:228:ALA:CB	1:C:231:ILE:HD11	0.57	2.28	8	1
1:D:275:VAL:HG22	1:E:239:VAL:CG1	0.57	2.28	10	2
1:D:231:ILE:HG22	1:D:239:VAL:HG11	0.57	1.74	15	1
1:E:265:GLU:N	1:E:265:GLU:CD	0.57	2.58	12	5
1:A:276:LEU:HD23	1:A:287:TRP:CZ2	0.57	2.34	11	2
1:B:276:LEU:HD13	1:B:287:TRP:CD2	0.57	2.35	4	1
1:A:264:VAL:HG23	1:B:231:ILE:HD11	0.57	1.77	8	2
1:C:240:GLN:HB3	1:C:276:LEU:HD22	0.57	1.76	5	2
1:C:280:GLU:CG	1:D:244:VAL:HG13	0.57	2.30	3	1
1:E:228:ALA:HB2	1:E:241:LEU:HD21	0.57	1.75	6	1
1:E:233:THR:OG1	1:E:237:ALA:HB3	0.57	1.98	20	2
1:A:280:GLU:HG2	1:B:244:VAL:HG12	0.57	1.77	8	2
1:D:240:GLN:O	1:D:241:LEU:HD22	0.57	1.99	5	2
1:A:231:ILE:HG22	1:A:267:VAL:CG2	0.57	2.29	16	4
1:A:233:THR:CB	1:A:237:ALA:HB3	0.57	2.29	20	4
1:E:239:VAL:HG12	1:E:275:VAL:CG2	0.57	2.30	16	4
1:D:226:ASN:ND2	1:D:277:ILE:HG22	0.56	2.14	20	1
1:B:286:PHE:CE1	1:C:276:LEU:HD21	0.56	2.35	10	1
1:A:239:VAL:HG12	1:A:275:VAL:HB	0.56	1.76	6	9
1:B:280:GLU:HG3	1:C:244:VAL:HG23	0.56	1.78	4	2
1:A:225:ARG:O	1:A:261:THR:HG23	0.56	2.01	5	3
1:C:233:THR:CB	1:C:237:ALA:HB3	0.56	2.30	20	2
1:C:239:VAL:HG12	1:C:275:VAL:CG2	0.56	2.30	7	2
1:C:276:LEU:HD12	1:C:287:TRP:CE3	0.56	2.35	14	1
1:A:275:VAL:HG13	1:B:239:VAL:HG23	0.56	1.78	13	2
1:E:233:THR:CB	1:E:237:ALA:HB3	0.56	2.31	20	2
1:B:231:ILE:HG22	1:B:267:VAL:HG12	0.56	1.76	19	1
1:A:225:ARG:HB3	1:A:261:THR:HG23	0.56	1.78	4	1
1:A:280:GLU:CG	1:B:244:VAL:HG23	0.56	2.31	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:267:VAL:HG23	1:C:231:ILE:HB	0.56	1.78	19	1
1:D:233:THR:OG1	1:D:237:ALA:HB3	0.55	2.00	20	2
1:B:225:ARG:HB2	1:B:261:THR:HG23	0.55	1.76	2	1
1:D:276:LEU:HD23	1:D:287:TRP:CZ2	0.55	2.37	12	2
1:B:264:VAL:HG23	1:C:228:ALA:HB3	0.55	1.78	6	4
1:B:275:VAL:HG12	1:B:277:ILE:HD11	0.55	1.78	7	2
1:D:233:THR:CB	1:D:237:ALA:HB3	0.55	2.30	20	3
1:B:231:ILE:HG21	1:B:239:VAL:HG21	0.55	1.77	10	1
1:C:277:ILE:CD1	1:D:241:LEU:HD13	0.55	2.31	12	1
1:B:260:THR:HG23	1:C:225:ARG:HB3	0.55	1.77	18	1
1:A:280:GLU:CD	1:B:244:VAL:HG13	0.55	2.22	15	1
1:A:275:VAL:HG22	1:B:239:VAL:CG2	0.55	2.31	18	1
1:C:264:VAL:HG21	1:C:267:VAL:HG12	0.55	1.77	7	1
1:B:280:GLU:CG	1:C:244:VAL:HG12	0.55	2.32	16	5
1:B:275:VAL:HG22	1:C:239:VAL:CG2	0.55	2.30	18	2
1:D:241:LEU:HD22	1:D:277:ILE:HD13	0.55	1.78	15	1
1:D:264:VAL:HG23	1:E:231:ILE:HD11	0.55	1.77	16	1
1:A:245:VAL:HG12	1:A:281:TYR:HB2	0.55	1.79	16	2
1:B:280:GLU:HG3	1:C:244:VAL:HG12	0.55	1.78	12	3
1:C:275:VAL:HG22	1:D:239:VAL:CG2	0.55	2.31	18	2
1:B:264:VAL:HA	1:C:228:ALA:HB3	0.55	1.76	18	1
1:D:240:GLN:HB3	1:D:276:LEU:HD13	0.55	1.78	10	2
1:B:225:ARG:HB3	1:B:261:THR:HG23	0.55	1.77	16	4
1:C:262:ASN:HB2	1:D:241:LEU:HD12	0.55	1.79	4	1
1:D:233:THR:HB	1:D:237:ALA:HB3	0.55	1.77	18	3
1:A:264:VAL:HG21	1:A:267:VAL:CG2	0.54	2.31	17	6
1:A:226:ASN:HB3	1:A:277:ILE:HG22	0.54	1.77	12	2
1:D:276:LEU:HD12	1:D:287:TRP:CG	0.54	2.36	13	1
1:A:280:GLU:HB3	1:B:244:VAL:HG23	0.54	1.79	6	1
1:D:264:VAL:HG23	1:E:231:ILE:CD1	0.54	2.32	17	3
1:C:277:ILE:HG13	1:D:241:LEU:HD23	0.54	1.79	17	1
1:B:276:LEU:HD12	1:B:287:TRP:CE2	0.54	2.38	8	1
1:D:228:ALA:HB2	1:D:241:LEU:HD11	0.54	1.79	15	1
1:B:280:GLU:HB2	1:C:244:VAL:HG23	0.54	1.80	6	1
1:B:264:VAL:HG22	1:C:241:LEU:HD22	0.54	1.78	9	1
1:D:277:ILE:HG13	1:E:241:LEU:HD23	0.54	1.80	3	1
1:B:249:ALA:HB2	1:B:281:TYR:CD1	0.54	2.37	5	2
1:A:283:GLY:H	1:B:247:ALA:HB2	0.54	1.62	20	2
1:D:275:VAL:HG22	1:E:239:VAL:HG22	0.54	1.77	13	1
1:D:277:ILE:CD1	1:E:241:LEU:HD13	0.54	2.32	6	2
1:D:239:VAL:HG12	1:D:275:VAL:CG2	0.54	2.33	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:277:ILE:CD1	1:D:241:LEU:HD23	0.53	2.29	1	2
1:C:275:VAL:HG13	1:D:239:VAL:HG23	0.53	1.79	2	3
1:A:233:THR:HG21	1:A:239:VAL:CG1	0.53	2.33	7	3
1:E:262:ASN:ND2	1:E:277:ILE:HG23	0.53	2.19	9	1
1:E:240:GLN:O	1:E:241:LEU:HD13	0.53	2.03	13	2
1:D:231:ILE:HG22	1:D:267:VAL:CG2	0.53	2.32	16	1
1:B:275:VAL:HG12	1:B:277:ILE:CD1	0.53	2.33	19	2
1:B:225:ARG:HG2	1:B:261:THR:HG23	0.53	1.81	15	1
1:A:262:ASN:CB	1:B:241:LEU:HD12	0.53	2.33	4	1
1:C:233:THR:HG21	1:C:239:VAL:HG13	0.53	1.79	6	3
1:D:275:VAL:HG22	1:E:239:VAL:CG2	0.53	2.33	13	3
1:E:229:LYS:N	1:E:229:LYS:HE3	0.53	2.19	14	1
1:D:226:ASN:HB3	1:D:277:ILE:HG22	0.53	1.79	1	2
1:D:276:LEU:HD12	1:D:287:TRP:CE2	0.53	2.39	16	1
1:E:275:VAL:O	1:E:276:LEU:HD22	0.53	2.03	11	1
1:E:229:LYS:HD2	1:E:230:ASP:N	0.53	2.19	14	1
1:C:241:LEU:HD12	1:C:277:ILE:CD1	0.53	2.32	7	1
1:E:241:LEU:HD12	1:E:277:ILE:CB	0.52	2.33	8	1
1:B:241:LEU:CD2	1:B:277:ILE:HD13	0.52	2.34	13	2
1:D:280:GLU:HG3	1:E:244:VAL:HG13	0.52	1.81	3	2
1:B:226:ASN:ND2	1:B:277:ILE:HG22	0.52	2.20	5	1
1:B:264:VAL:HG21	1:B:277:ILE:CD1	0.52	2.28	9	1
1:B:264:VAL:HG11	1:B:267:VAL:CG2	0.52	2.34	9	1
1:C:281:TYR:OH	1:D:249:ALA:HB2	0.52	2.04	2	1
1:B:233:THR:HG21	1:B:239:VAL:CG1	0.52	2.35	7	2
1:D:283:GLY:CA	1:E:247:ALA:HB2	0.52	2.35	1	1
1:C:233:THR:HB	1:C:237:ALA:HB3	0.52	1.81	18	3
1:D:241:LEU:CD1	1:D:277:ILE:HD12	0.52	2.31	17	1
1:C:264:VAL:HG21	1:C:267:VAL:CG2	0.52	2.35	8	8
1:C:232:ARG:HD2	1:C:268:VAL:HG22	0.52	1.82	5	1
1:C:280:GLU:OE2	1:D:244:VAL:HG13	0.52	2.04	5	1
1:A:280:GLU:OE1	1:B:244:VAL:HG13	0.52	2.05	15	1
1:C:276:LEU:HD23	1:C:287:TRP:CZ2	0.52	2.39	12	3
1:B:260:THR:HG21	1:C:243:ASN:ND2	0.52	2.19	5	1
1:D:267:VAL:CG1	1:D:275:VAL:HG11	0.52	2.30	6	1
1:B:276:LEU:HD23	1:B:287:TRP:CZ2	0.52	2.39	15	2
1:C:264:VAL:HA	1:D:228:ALA:HB3	0.52	1.82	19	1
1:B:280:GLU:CG	1:C:244:VAL:HG23	0.51	2.35	4	2
1:D:283:GLY:N	1:E:247:ALA:HB2	0.51	2.20	16	3
1:A:239:VAL:HG12	1:A:275:VAL:CG2	0.51	2.35	7	3
1:A:232:ARG:HD2	1:A:268:VAL:HG22	0.51	1.81	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:264:VAL:HG21	1:D:277:ILE:CD1	0.51	2.35	9	1
1:B:249:ALA:HB2	1:B:282:GLY:HA3	0.51	1.83	6	2
1:E:240:GLN:O	1:E:241:LEU:HD22	0.51	2.05	2	1
1:A:264:VAL:HG21	1:B:231:ILE:HD11	0.51	1.81	12	2
1:C:264:VAL:HG21	1:C:267:VAL:HG22	0.51	1.81	8	4
1:B:264:VAL:CG2	1:B:277:ILE:HD12	0.51	2.30	9	1
1:C:264:VAL:CG2	1:C:277:ILE:HD12	0.51	2.35	9	1
1:E:229:LYS:HD3	1:E:265:GLU:O	0.51	2.05	14	1
1:E:239:VAL:HG23	1:E:275:VAL:HB	0.51	1.83	17	2
1:E:240:GLN:O	1:E:276:LEU:HD23	0.51	2.06	9	1
1:B:267:VAL:HG13	1:C:231:ILE:CD1	0.51	2.36	4	1
1:D:267:VAL:HG22	1:E:231:ILE:HD11	0.51	1.83	4	1
1:E:225:ARG:O	1:E:261:THR:HG22	0.51	2.06	8	1
1:D:280:GLU:CD	1:E:244:VAL:HG13	0.50	2.27	11	2
1:B:264:VAL:HG21	1:B:267:VAL:HG22	0.50	1.83	14	6
1:A:225:ARG:HG3	1:A:261:THR:HG23	0.50	1.83	10	3
1:C:240:GLN:C	1:C:241:LEU:HD22	0.50	2.27	5	1
1:A:232:ARG:HD3	1:A:268:VAL:HG22	0.50	1.84	6	1
1:C:260:THR:HG21	1:C:279:ASN:CB	0.50	2.37	9	1
1:C:230:ASP:HB3	1:C:266:THR:HG22	0.50	1.81	18	2
1:C:277:ILE:HD12	1:D:241:LEU:HD22	0.50	1.83	16	1
1:A:264:VAL:HG21	1:A:267:VAL:HG22	0.50	1.82	20	8
1:C:230:ASP:CB	1:C:266:THR:HG22	0.50	2.36	10	1
1:C:261:THR:HG23	1:D:225:ARG:CB	0.50	2.35	10	1
1:B:277:ILE:HD13	1:C:241:LEU:HD13	0.50	1.81	16	1
1:C:226:ASN:HB3	1:C:277:ILE:HG22	0.50	1.82	1	1
1:B:240:GLN:HB3	1:B:276:LEU:HD22	0.50	1.83	5	3
1:E:233:THR:HG21	1:E:239:VAL:CG1	0.50	2.36	12	2
1:E:230:ASP:HB2	1:E:266:THR:HG22	0.50	1.83	12	3
1:B:280:GLU:HG3	1:C:244:VAL:HG13	0.50	1.82	18	2
1:C:246:THR:HG23	1:C:281:TYR:O	0.50	2.07	17	1
1:D:230:ASP:HB3	1:D:266:THR:HG23	0.50	1.84	18	2
1:D:246:THR:HG22	1:D:282:GLY:HA3	0.50	1.84	8	1
1:E:228:ALA:CB	1:E:231:ILE:HD11	0.50	2.36	8	1
1:D:264:VAL:HG21	1:D:267:VAL:CG2	0.50	2.37	14	10
1:E:240:GLN:HB3	1:E:276:LEU:HD22	0.50	1.81	2	2
1:D:233:THR:HG21	1:D:239:VAL:CG1	0.50	2.37	7	3
1:A:275:VAL:HG13	1:B:239:VAL:HG13	0.50	1.82	10	1
1:E:232:ARG:HD2	1:E:268:VAL:HG13	0.50	1.84	18	1
1:A:283:GLY:N	1:B:247:ALA:HB2	0.50	2.22	20	1
1:D:264:VAL:HG21	1:D:267:VAL:HG22	0.50	1.82	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:264:VAL:HG21	1:E:267:VAL:HG13	0.50	1.81	6	1
1:D:260:THR:HG23	1:E:225:ARG:HD2	0.50	1.84	7	2
1:A:231:ILE:HG23	1:A:267:VAL:HB	0.49	1.83	1	1
1:A:267:VAL:CG2	1:B:231:ILE:HD11	0.49	2.36	4	1
1:B:267:VAL:HG11	1:B:275:VAL:HG11	0.49	1.83	5	2
1:C:264:VAL:HG21	1:D:231:ILE:CD1	0.49	2.37	4	2
1:D:276:LEU:HD13	1:D:287:TRP:CE3	0.49	2.43	4	1
1:A:225:ARG:CB	1:A:261:THR:HG22	0.49	2.36	20	1
1:B:260:THR:HG22	1:C:225:ARG:NH1	0.49	2.22	15	1
1:C:233:THR:HG21	1:C:239:VAL:CG1	0.49	2.37	16	3
1:A:264:VAL:HG21	1:A:277:ILE:CD1	0.49	2.37	9	1
1:C:280:GLU:HG3	1:D:244:VAL:HG12	0.49	1.84	9	1
1:D:276:LEU:HD12	1:D:287:TRP:CD2	0.49	2.43	16	1
1:B:283:GLY:H	1:C:247:ALA:HB2	0.49	1.68	17	2
1:C:275:VAL:HG12	1:C:277:ILE:CD1	0.49	2.37	19	1
1:D:231:ILE:HD12	1:D:239:VAL:HG11	0.49	1.83	20	1
1:B:245:VAL:CG1	1:B:249:ALA:HB3	0.49	2.38	7	2
1:A:240:GLN:OE1	1:A:276:LEU:HD21	0.49	2.08	14	1
1:B:267:VAL:HG13	1:C:231:ILE:HD12	0.49	1.85	4	1
1:A:281:TYR:CZ	1:B:245:VAL:HG11	0.49	2.43	8	1
1:B:233:THR:HB	1:B:237:ALA:HB3	0.49	1.84	18	4
1:B:280:GLU:CD	1:C:244:VAL:HG13	0.48	2.28	3	1
1:A:276:LEU:O	1:B:241:LEU:HD12	0.48	2.08	7	1
1:C:264:VAL:HG21	1:C:277:ILE:CD1	0.48	2.36	9	1
1:A:231:ILE:HG21	1:A:275:VAL:HG11	0.48	1.85	1	1
1:D:264:VAL:HG11	1:D:267:VAL:CG2	0.48	2.39	9	1
1:E:264:VAL:O	1:E:264:VAL:HG13	0.48	2.08	15	1
1:E:241:LEU:CD2	1:E:277:ILE:HD13	0.48	2.39	15	1
1:E:267:VAL:HG21	1:E:275:VAL:HG21	0.48	1.84	19	1
1:D:275:VAL:HG12	1:D:277:ILE:HD11	0.48	1.86	3	1
1:B:280:GLU:HG2	1:C:244:VAL:HG12	0.48	1.86	16	2
1:C:249:ALA:HB1	1:C:281:TYR:CD2	0.48	2.44	11	1
1:D:228:ALA:CB	1:D:231:ILE:HD11	0.48	2.39	1	1
1:E:231:ILE:HG23	1:E:267:VAL:HG11	0.48	1.85	14	1
1:A:275:VAL:HG22	1:B:239:VAL:HG22	0.48	1.86	18	1
1:E:233:THR:HB	1:E:237:ALA:HB3	0.48	1.85	20	2
1:B:231:ILE:HG22	1:B:267:VAL:CG2	0.48	2.39	12	1
1:E:229:LYS:CD	1:E:230:ASP:N	0.48	2.77	14	1
1:B:267:VAL:HG12	1:C:231:ILE:CD1	0.48	2.39	16	1
1:C:245:VAL:HG12	1:C:281:TYR:CB	0.48	2.39	6	1
1:D:264:VAL:HG23	1:E:231:ILE:HD13	0.48	1.85	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:231:ILE:CG2	1:D:239:VAL:HG11	0.48	2.38	15	1
1:A:239:VAL:HG12	1:A:275:VAL:CB	0.47	2.38	6	3
1:D:275:VAL:HG22	1:E:239:VAL:HG12	0.47	1.85	17	2
1:A:241:LEU:HD12	1:A:277:ILE:HG13	0.47	1.85	1	1
1:C:225:ARG:O	1:C:261:THR:HG23	0.47	2.09	16	2
1:B:231:ILE:HD12	1:B:239:VAL:HG21	0.47	1.86	20	1
1:E:264:VAL:HG21	1:E:267:VAL:CG1	0.47	2.39	6	1
1:A:233:THR:HB	1:A:237:ALA:HB3	0.47	1.85	20	4
1:B:276:LEU:HD23	1:C:240:GLN:CG	0.47	2.39	20	1
1:C:280:GLU:HG2	1:D:244:VAL:HG22	0.47	1.86	5	2
1:E:264:VAL:HG21	1:E:267:VAL:HG22	0.47	1.85	7	1
1:B:275:VAL:HG13	1:C:239:VAL:HG23	0.47	1.85	13	3
1:D:276:LEU:HD23	1:E:240:GLN:HG2	0.47	1.86	4	1
1:E:230:ASP:HB3	1:E:266:THR:HG23	0.47	1.86	4	1
1:A:264:VAL:CG1	1:A:267:VAL:HG23	0.47	2.40	9	1
1:D:245:VAL:HG13	1:D:281:TYR:HB3	0.47	1.86	14	2
1:B:282:GLY:O	1:C:247:ALA:HB2	0.47	2.10	11	1
1:E:264:VAL:HG22	1:E:266:THR:H	0.47	1.69	14	1
1:C:241:LEU:HD22	1:C:241:LEU:N	0.47	2.25	1	3
1:A:235:GLU:O	1:A:236:ARG:C	0.47	2.52	2	3
1:D:261:THR:H	1:E:225:ARG:NE	0.47	2.06	10	1
1:C:282:GLY:O	1:D:247:ALA:HB2	0.47	2.10	11	2
1:A:231:ILE:HG22	1:A:267:VAL:HG12	0.47	1.85	19	1
1:A:262:ASN:HB2	1:B:241:LEU:HD12	0.47	1.87	4	1
1:C:245:VAL:HG13	1:C:249:ALA:HB3	0.47	1.86	7	1
1:D:262:ASN:OD1	1:D:277:ILE:HG23	0.47	2.09	11	1
1:E:235:GLU:O	1:E:236:ARG:C	0.47	2.52	7	1
1:A:260:THR:HG23	1:B:225:ARG:N	0.47	2.25	10	1
1:C:264:VAL:CG2	1:D:231:ILE:HD11	0.47	2.40	16	1
1:B:241:LEU:HD12	1:B:277:ILE:HB	0.46	1.86	3	2
1:B:276:LEU:HD12	1:B:287:TRP:NE1	0.46	2.25	8	1
1:B:262:ASN:OD1	1:C:241:LEU:HD12	0.46	2.10	6	1
1:E:240:GLN:C	1:E:241:LEU:HD13	0.46	2.31	20	2
1:A:246:THR:HG21	1:A:284:LYS:HB2	0.46	1.86	17	1
1:C:231:ILE:HD12	1:C:239:VAL:HG11	0.46	1.87	20	1
1:B:262:ASN:ND2	1:B:277:ILE:HG22	0.46	2.25	10	1
1:B:276:LEU:HD12	1:B:287:TRP:CZ2	0.46	2.45	18	1
1:D:286:PHE:HE1	1:E:244:VAL:HG21	0.46	1.71	1	1
1:C:225:ARG:N	1:C:261:THR:HG23	0.46	2.26	1	1
1:C:231:ILE:HG22	1:C:267:VAL:HG21	0.46	1.86	4	1
1:B:231:ILE:HD12	1:B:239:VAL:HG11	0.46	1.87	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:245:VAL:HG12	1:B:281:TYR:HB2	0.46	1.86	6	1
1:E:265:GLU:N	1:E:265:GLU:OE1	0.46	2.48	15	2
1:E:230:ASP:CB	1:E:266:THR:HG22	0.46	2.41	3	3
1:C:231:ILE:CD1	1:C:241:LEU:HD21	0.46	2.41	17	1
1:B:239:VAL:HG12	1:B:275:VAL:CG2	0.46	2.41	7	1
1:A:275:VAL:HG12	1:A:277:ILE:CD1	0.46	2.40	19	1
1:A:241:LEU:HD12	1:A:277:ILE:CG1	0.46	2.41	1	1
1:A:276:LEU:HD12	1:A:287:TRP:CZ2	0.46	2.45	8	1
1:E:264:VAL:HG11	1:E:267:VAL:CG2	0.46	2.41	9	1
1:D:280:GLU:CG	1:E:244:VAL:HG23	0.46	2.40	4	1
1:E:225:ARG:HA	1:E:261:THR:HG23	0.46	1.88	4	1
1:C:260:THR:HG21	1:D:243:ASN:CG	0.46	2.31	10	1
1:E:264:VAL:HG21	1:E:267:VAL:CG2	0.45	2.42	1	3
1:C:267:VAL:HG11	1:C:275:VAL:CG1	0.45	2.40	6	1
1:C:261:THR:HG23	1:D:225:ARG:HB3	0.45	1.86	13	2
1:D:241:LEU:HD21	1:D:277:ILE:HD12	0.45	1.87	13	2
1:E:239:VAL:HG12	1:E:275:VAL:CB	0.45	2.41	16	1
1:B:241:LEU:HD22	1:B:241:LEU:N	0.45	2.27	1	1
1:C:245:VAL:CG1	1:C:249:ALA:HB3	0.45	2.42	7	3
1:C:260:THR:HG21	1:D:243:ASN:HB3	0.45	1.86	1	1
1:D:225:ARG:N	1:D:261:THR:HG23	0.45	2.25	13	4
1:A:231:ILE:HG22	1:A:267:VAL:HG23	0.45	1.87	16	1
1:C:231:ILE:HG22	1:C:267:VAL:HG23	0.45	1.87	6	2
1:C:243:ASN:ND2	1:C:245:VAL:HG23	0.45	2.26	7	1
1:E:246:THR:HG21	1:E:282:GLY:C	0.45	2.32	18	1
1:A:267:VAL:HG13	1:B:231:ILE:CG1	0.45	2.41	16	1
1:B:260:THR:HG23	1:C:225:ARG:CB	0.45	2.42	18	1
1:D:241:LEU:HD22	1:D:241:LEU:N	0.45	2.26	1	2
1:D:241:LEU:HD13	1:D:277:ILE:CB	0.45	2.40	15	2
1:B:249:ALA:HB2	1:B:282:GLY:CA	0.45	2.41	6	2
1:A:244:VAL:HG23	1:A:244:VAL:O	0.45	2.12	16	1
1:B:260:THR:HG21	1:C:243:ASN:HB2	0.45	1.89	12	1
1:D:260:THR:HG21	1:E:243:ASN:OD1	0.45	2.12	18	1
1:D:264:VAL:CG2	1:D:277:ILE:HD12	0.45	2.40	9	1
1:A:276:LEU:HD23	1:A:287:TRP:HZ2	0.45	1.71	11	1
1:C:239:VAL:HG23	1:C:275:VAL:HB	0.45	1.87	19	2
1:E:264:VAL:HG21	1:E:277:ILE:CD1	0.45	2.37	13	1
1:D:225:ARG:H	1:D:261:THR:HG23	0.45	1.72	14	1
1:C:226:ASN:OD1	1:C:277:ILE:HG22	0.45	2.12	16	1
1:B:246:THR:HG22	1:B:282:GLY:HA3	0.45	1.89	17	1
1:D:241:LEU:CD2	1:D:277:ILE:HD12	0.45	2.42	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:229:LYS:HE2	1:E:265:GLU:C	0.45	2.32	14	1
1:D:260:THR:HG23	1:E:225:ARG:HG2	0.44	1.88	5	1
1:D:246:THR:HG23	1:D:248:ALA:H	0.44	1.73	5	1
1:D:280:GLU:HG3	1:E:244:VAL:HG12	0.44	1.87	2	1
1:D:275:VAL:C	1:D:276:LEU:HD23	0.44	2.33	6	1
1:D:245:VAL:HG13	1:D:281:TYR:CB	0.44	2.43	10	1
1:E:231:ILE:CG2	1:E:239:VAL:HG21	0.44	2.43	19	2
1:D:264:VAL:CG2	1:E:241:LEU:HD22	0.44	2.38	12	1
1:B:240:GLN:C	1:B:241:LEU:HD23	0.44	2.33	17	1
1:E:241:LEU:HD23	1:E:264:VAL:HG11	0.44	1.88	17	1
1:D:283:GLY:HA3	1:E:247:ALA:HB2	0.44	1.90	1	1
1:A:240:GLN:HB3	1:A:276:LEU:HD22	0.44	1.89	6	1
1:E:231:ILE:HG23	1:E:267:VAL:HG23	0.44	1.89	6	1
1:E:231:ILE:HG21	1:E:239:VAL:HG11	0.44	1.90	17	1
1:D:276:LEU:HD12	1:D:287:TRP:HE1	0.44	1.72	18	1
1:A:277:ILE:CD1	1:B:241:LEU:HD23	0.44	2.43	1	1
1:E:233:THR:HG21	1:E:239:VAL:HG13	0.44	1.88	16	1
1:A:245:VAL:HG12	1:A:281:TYR:HB3	0.44	1.87	6	1
1:C:280:GLU:HG3	1:D:244:VAL:HG23	0.44	1.87	4	1
1:D:275:VAL:O	1:D:276:LEU:HD22	0.44	2.13	7	1
1:B:231:ILE:CG2	1:B:239:VAL:HG21	0.44	2.43	10	1
1:B:277:ILE:CD1	1:C:241:LEU:HD23	0.44	2.30	1	1
1:C:262:ASN:HD21	1:C:277:ILE:HG23	0.44	1.73	12	1
1:D:276:LEU:HD23	1:D:287:TRP:CE2	0.43	2.48	5	1
1:B:262:ASN:ND2	1:B:277:ILE:HG23	0.43	2.28	6	1
1:C:248:ALA:O	1:C:249:ALA:HB3	0.43	2.12	9	1
1:C:225:ARG:HA	1:C:261:THR:HG23	0.43	1.88	20	2
1:B:286:PHE:CE2	1:C:244:VAL:HG21	0.43	2.48	12	1
1:D:241:LEU:HD12	1:D:277:ILE:CD1	0.43	2.43	7	1
1:B:280:GLU:OE1	1:C:244:VAL:HG13	0.43	2.14	15	1
1:B:264:VAL:HG21	1:B:267:VAL:CG2	0.43	2.44	17	7
1:E:246:THR:HG22	1:E:281:TYR:CD1	0.43	2.48	18	1
1:B:275:VAL:HG22	1:C:239:VAL:HG22	0.43	1.90	18	2
1:C:231:ILE:HD11	1:C:241:LEU:HD21	0.43	1.91	17	1
1:B:283:GLY:N	1:C:247:ALA:HB2	0.43	2.28	15	3
1:C:262:ASN:HB2	1:C:277:ILE:HG22	0.43	1.89	3	1
1:C:267:VAL:HG22	1:D:231:ILE:HB	0.43	1.90	19	1
1:D:233:THR:HG21	1:D:239:VAL:HG13	0.43	1.91	6	1
1:B:245:VAL:HG12	1:B:281:TYR:HB3	0.43	1.90	6	1
1:D:282:GLY:O	1:E:247:ALA:HB2	0.43	2.14	12	1
1:D:281:TYR:CE2	1:E:249:ALA:HB2	0.43	2.49	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:275:VAL:CG1	1:B:277:ILE:HD11	0.43	2.43	7	1
1:A:233:THR:HG21	1:A:239:VAL:HG13	0.43	1.90	16	1
1:D:264:VAL:HG11	1:D:277:ILE:CD1	0.43	2.44	17	1
1:A:239:VAL:HG23	1:A:275:VAL:HB	0.43	1.91	19	1
1:B:260:THR:HG21	1:C:243:ASN:H	0.43	1.73	19	1
1:C:230:ASP:HB3	1:C:266:THR:HG23	0.43	1.91	1	2
1:C:276:LEU:O	1:D:241:LEU:HD22	0.43	2.14	7	1
1:A:225:ARG:CG	1:A:261:THR:HG23	0.42	2.44	3	1
1:A:277:ILE:HD13	1:B:241:LEU:HD13	0.42	1.89	5	3
1:D:260:THR:HG22	1:D:262:ASN:OD1	0.42	2.13	7	1
1:E:241:LEU:HD22	1:E:277:ILE:CB	0.42	2.43	10	1
1:A:231:ILE:HG22	1:A:267:VAL:HG22	0.42	1.89	6	1
1:A:231:ILE:HG22	1:A:267:VAL:HG21	0.42	1.91	12	1
1:A:267:VAL:HG12	1:B:231:ILE:HG12	0.42	1.91	6	1
1:C:267:VAL:HG13	1:D:231:ILE:HD12	0.42	1.91	6	1
1:D:262:ASN:ND2	1:D:277:ILE:HG23	0.42	2.29	9	1
1:D:240:GLN:C	1:D:241:LEU:HD22	0.42	2.35	19	1
1:D:262:ASN:OD1	1:E:241:LEU:HD12	0.42	2.14	19	1
1:D:286:PHE:HB3	1:E:244:VAL:HG11	0.42	1.91	20	1
1:B:260:THR:HG23	1:C:225:ARG:CG	0.42	2.44	3	1
1:B:246:THR:HG23	1:B:281:TYR:O	0.42	2.14	10	1
1:B:283:GLY:HA3	1:C:247:ALA:HB2	0.42	1.92	15	1
1:D:267:VAL:HG11	1:D:275:VAL:CG2	0.42	2.43	15	1
1:B:276:LEU:HD22	1:B:287:TRP:CE2	0.42	2.49	20	1
1:B:267:VAL:CG1	1:B:275:VAL:HG11	0.42	2.44	10	1
1:E:267:VAL:HG11	1:E:275:VAL:CG2	0.42	2.35	10	2
1:D:275:VAL:HG12	1:D:277:ILE:CD1	0.42	2.45	3	1
1:A:285:GLY:O	1:B:244:VAL:HG11	0.42	2.13	7	1
1:B:260:THR:HG23	1:C:225:ARG:CD	0.42	2.45	3	1
1:C:241:LEU:HD22	1:C:277:ILE:HB	0.42	1.90	4	1
1:E:229:LYS:HD2	1:E:230:ASP:CB	0.42	2.44	14	1
1:B:267:VAL:HG12	1:C:231:ILE:HG12	0.42	1.91	6	1
1:C:241:LEU:HD13	1:C:241:LEU:N	0.42	2.30	1	1
1:D:226:ASN:OD1	1:D:277:ILE:HG22	0.42	2.14	16	1
1:E:226:ASN:HB3	1:E:277:ILE:HG22	0.42	1.90	1	1
1:C:281:TYR:CZ	1:D:245:VAL:HG11	0.42	2.49	7	1
1:C:280:GLU:OE1	1:D:244:VAL:HG13	0.42	2.15	15	1
1:C:240:GLN:OE1	1:C:276:LEU:HD21	0.42	2.15	16	1
1:B:277:ILE:CG1	1:C:241:LEU:HD13	0.42	2.44	17	1
1:B:235:GLU:O	1:B:236:ARG:C	0.41	2.57	10	2
1:D:280:GLU:OE2	1:E:244:VAL:HG13	0.41	2.15	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:246:THR:HG21	1:A:284:LYS:CB	0.41	2.44	17	1
1:D:281:TYR:OH	1:E:249:ALA:HB2	0.41	2.15	1	1
1:D:231:ILE:HG21	1:D:275:VAL:HG11	0.41	1.92	8	1
1:B:231:ILE:HG22	1:B:267:VAL:HG21	0.41	1.92	12	1
1:C:249:ALA:HB2	1:C:281:TYR:CE1	0.41	2.50	2	1
1:C:260:THR:HG21	1:D:243:ASN:CB	0.41	2.45	8	1
1:D:249:ALA:HB1	1:D:281:TYR:CE2	0.41	2.51	8	1
1:B:228:ALA:HB2	1:B:241:LEU:HD21	0.41	1.91	20	1
1:B:286:PHE:HA	1:C:244:VAL:HG21	0.41	1.91	6	1
1:E:265:GLU:CG	1:E:266:THR:N	0.41	2.83	17	2
1:A:283:GLY:H	1:B:247:ALA:N	0.41	2.13	15	1
1:D:231:ILE:HG23	1:D:267:VAL:HB	0.41	1.91	8	1
1:B:244:VAL:O	1:B:244:VAL:HG23	0.41	2.15	16	1
1:A:267:VAL:HG23	1:B:231:ILE:HG13	0.41	1.91	19	1
1:D:239:VAL:HG23	1:D:275:VAL:CG1	0.41	2.46	1	1
1:C:276:LEU:HD12	1:C:287:TRP:HE1	0.41	1.75	18	1
1:B:239:VAL:HG23	1:B:275:VAL:HB	0.41	1.92	1	2
1:E:229:LYS:HE3	1:E:229:LYS:H	0.41	1.75	14	1
1:C:241:LEU:HD21	1:C:277:ILE:HD13	0.41	1.93	20	1
1:A:240:GLN:OE1	1:A:276:LEU:HD11	0.41	2.16	3	1
1:C:260:THR:HG23	1:D:225:ARG:CB	0.41	2.44	20	1
1:B:262:ASN:HB2	1:B:277:ILE:HG22	0.41	1.92	3	1
1:D:241:LEU:HD22	1:D:277:ILE:HB	0.41	1.93	4	1
1:E:264:VAL:CG2	1:E:267:VAL:HG13	0.41	2.46	6	1
1:A:262:ASN:HD22	1:B:241:LEU:HD23	0.41	1.75	8	1
1:C:249:ALA:HB1	1:C:281:TYR:CE2	0.41	2.51	11	1
1:A:275:VAL:HG12	1:A:277:ILE:HD11	0.41	1.93	19	1
1:D:241:LEU:HD13	1:D:241:LEU:N	0.41	2.31	7	1
1:D:276:LEU:HD23	1:D:287:TRP:HZ2	0.41	1.75	12	1
1:B:241:LEU:HD22	1:B:277:ILE:CD1	0.41	2.46	17	1
1:E:265:GLU:CD	1:E:265:GLU:C	0.40	2.80	13	1
1:A:260:THR:HG21	1:A:279:ASN:HB3	0.40	1.94	17	1
1:A:282:GLY:O	1:B:247:ALA:HB2	0.40	2.16	3	1
1:B:240:GLN:OE1	1:B:276:LEU:HD11	0.40	2.17	10	1
1:D:246:THR:HG23	1:D:281:TYR:O	0.40	2.16	12	1
1:D:276:LEU:HD13	1:D:287:TRP:CZ2	0.40	2.51	20	1
1:D:284:LYS:N	1:E:246:THR:HG23	0.40	2.32	4	1
1:B:230:ASP:HB3	1:B:266:THR:HG23	0.40	1.93	10	1
1:B:240:GLN:O	1:B:277:ILE:HD12	0.40	2.15	13	1
1:C:260:THR:HG21	1:C:279:ASN:CG	0.40	2.37	9	1
1:E:240:GLN:C	1:E:241:LEU:HD12	0.40	2.37	11	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	50/79 (63%)	42±1 (84±2%)	6±2 (12±3%)	2±1 (4±2%)	4	28
1	B	54/79 (68%)	45±2 (84±4%)	6±2 (12±3%)	2±1 (4±2%)	5	31
1	C	54/79 (68%)	46±2 (84±3%)	6±2 (11±3%)	3±1 (5±2%)	4	26
1	D	53/79 (67%)	44±2 (84±3%)	6±2 (11±3%)	3±1 (5±2%)	3	23
1	E	47/79 (59%)	41±1 (87±2%)	4±1 (9±3%)	2±1 (5±2%)	4	27
All	All	5160/7900 (65%)	4362 (85%)	556 (11%)	242 (5%)	4	27

All 50 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	271	GLY	15
1	B	271	GLY	13
1	C	271	GLY	13
1	D	271	GLY	13
1	E	271	GLY	13
1	E	265	GLU	10
1	C	287	TRP	8
1	A	287	TRP	8
1	D	286	PHE	7
1	D	249	ALA	7
1	E	249	ALA	7
1	D	284	LYS	6
1	A	286	PHE	6
1	C	284	LYS	6
1	E	272	GLU	6
1	C	272	GLU	6
1	B	285	GLY	5
1	C	249	ALA	5
1	D	285	GLY	5
1	D	272	GLU	5
1	A	285	GLY	4
1	B	259	GLN	4

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Mol	Chain	Res	Type	Models (Total)
1	D	287	TRP	4
1	C	286	PHE	4
1	B	284	LYS	4
1	A	236	ARG	4
1	B	236	ARG	4
1	C	259	GLN	3
1	A	283	GLY	3
1	E	225	ARG	3
1	B	286	PHE	3
1	B	287	TRP	3
1	B	272	GLU	3
1	C	236	ARG	3
1	C	285	GLY	3
1	D	236	ARG	3
1	E	236	ARG	3
1	D	225	ARG	2
1	B	249	ALA	2
1	D	265	GLU	2
1	A	272	GLU	2
1	C	225	ARG	2
1	D	282	GLY	2
1	A	284	LYS	2
1	E	282	GLY	1
1	A	225	ARG	1
1	B	225	ARG	1
1	D	235	GLU	1
1	D	283	GLY	1
1	B	283	GLY	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	41/63 (65%)	31±2 (75±6%)	10±2 (25±6%)	2 25
1	B	42/63 (67%)	30±3 (72±6%)	12±3 (28±6%)	2 20
1	C	42/63 (67%)	31±2 (73±4%)	11±2 (27±4%)	2 22
1	D	41/63 (65%)	30±3 (73±7%)	11±3 (27±7%)	2 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	37/63 (59%)	27±2 (73±6%)	10±2 (27±6%)	2 22
All	All	4060/6300 (64%)	2983 (73%)	1077 (27%)	2 22

All 175 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	C	276	LEU	19
1	B	229	LYS	17
1	B	276	LEU	17
1	A	276	LEU	16
1	C	229	LYS	15
1	E	229	LYS	15
1	A	284	LYS	14
1	D	225	ARG	14
1	D	276	LEU	14
1	E	276	LEU	14
1	B	227	SER	13
1	B	238	ARG	13
1	C	265	GLU	13
1	D	229	LYS	13
1	B	233	THR	13
1	A	229	LYS	12
1	A	270	LYS	12
1	A	233	THR	12
1	D	270	LYS	12
1	E	233	THR	12
1	E	265	GLU	12
1	E	230	ASP	12
1	C	225	ARG	11
1	C	259	GLN	11
1	C	233	THR	11
1	D	227	SER	11
1	E	227	SER	11
1	B	241	LEU	10
1	D	262	ASN	10
1	E	225	ARG	10
1	D	233	THR	10
1	D	265	GLU	10
1	B	225	ARG	10
1	C	262	ASN	10
1	D	263	SER	10

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Mol	Chain	Res	Type	Models (Total)
1	A	241	LEU	9
1	C	241	LEU	9
1	A	227	SER	9
1	B	262	ASN	9
1	B	274	ARG	9
1	C	230	ASP	9
1	B	284	LYS	9
1	D	238	ARG	8
1	E	236	ARG	8
1	E	263	SER	8
1	E	270	LYS	8
1	E	274	ARG	8
1	A	225	ARG	8
1	B	230	ASP	8
1	B	281	TYR	8
1	B	280	GLU	8
1	C	263	SER	8
1	A	281	TYR	8
1	C	235	GLU	8
1	A	238	ARG	8
1	D	235	GLU	8
1	B	235	GLU	8
1	C	227	SER	7
1	D	241	LEU	7
1	A	240	GLN	7
1	E	240	GLN	7
1	C	232	ARG	7
1	C	238	ARG	7
1	D	230	ASP	7
1	D	274	ARG	7
1	E	238	ARG	7
1	B	259	GLN	7
1	D	284	LYS	7
1	E	262	ASN	7
1	B	232	ARG	7
1	A	235	GLU	7
1	C	284	LYS	7
1	A	280	GLU	7
1	B	265	GLU	6
1	B	270	LYS	6
1	C	226	ASN	6
1	D	236	ARG	6

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Mol	Chain	Res	Type	Models (Total)
1	A	236	ARG	6
1	D	226	ASN	6
1	E	280	GLU	6
1	B	226	ASN	6
1	B	236	ARG	6
1	B	240	GLN	6
1	D	280	GLU	6
1	A	262	ASN	6
1	D	286	PHE	6
1	C	270	LYS	6
1	A	265	GLU	5
1	A	226	ASN	5
1	C	286	PHE	5
1	E	226	ASN	5
1	A	260	THR	5
1	E	261	THR	5
1	E	266	THR	5
1	A	274	ARG	5
1	C	240	GLN	5
1	A	273	SER	5
1	E	243	ASN	5
1	D	266	THR	4
1	A	286	PHE	4
1	C	234	GLU	4
1	D	240	GLN	4
1	E	232	ARG	4
1	C	274	ARG	4
1	C	280	GLU	4
1	E	281	TYR	4
1	A	232	ARG	4
1	B	286	PHE	4
1	C	273	SER	4
1	E	234	GLU	4
1	B	273	SER	4
1	B	287	TRP	4
1	C	267	VAL	4
1	D	287	TRP	4
1	C	236	ARG	4
1	C	260	THR	4
1	D	273	SER	4
1	A	246	THR	4
1	D	243	ASN	4

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Mol	Chain	Res	Type	Models (Total)
1	D	272	GLU	4
1	A	261	THR	4
1	D	232	ARG	4
1	E	241	LEU	4
1	C	272	GLU	4
1	D	260	THR	4
1	C	261	THR	3
1	C	266	THR	3
1	C	279	ASN	3
1	A	263	SER	3
1	E	273	SER	3
1	A	287	TRP	3
1	A	230	ASP	3
1	C	281	TYR	3
1	D	231	ILE	3
1	D	261	THR	3
1	A	266	THR	3
1	B	263	SER	3
1	B	279	ASN	3
1	B	234	GLU	3
1	B	260	THR	3
1	B	243	ASN	2
1	C	243	ASN	2
1	B	231	ILE	2
1	E	272	GLU	2
1	B	239	VAL	2
1	D	234	GLU	2
1	D	267	VAL	2
1	A	234	GLU	2
1	D	279	ASN	2
1	E	264	VAL	2
1	C	231	ILE	2
1	E	235	GLU	2
1	A	267	VAL	2
1	E	231	ILE	2
1	E	279	ASN	2
1	A	272	GLU	2
1	B	246	THR	1
1	A	239	VAL	1
1	C	239	VAL	1
1	D	281	TYR	1
1	B	267	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	E	244	VAL	1
1	D	244	VAL	1
1	D	264	VAL	1
1	B	261	THR	1
1	B	272	GLU	1
1	D	239	VAL	1
1	E	245	VAL	1
1	B	245	VAL	1
1	A	231	ILE	1
1	A	244	VAL	1
1	A	243	ASN	1
1	C	287	TRP	1
1	E	268	VAL	1
1	A	279	ASN	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided