



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 03:47 PM UTC

PDB ID : 2RNM / pdb_00002rnm
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 ⓘ 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

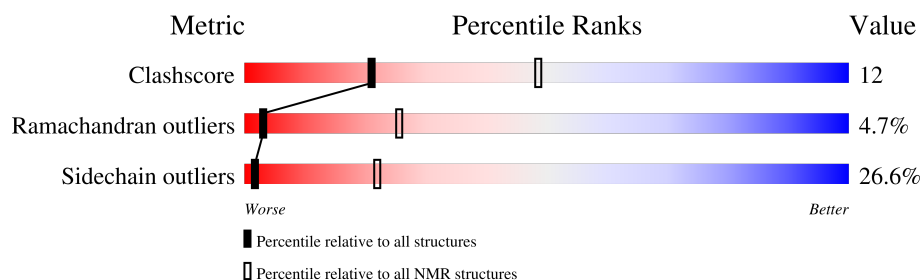
1 Overall quality at a glance

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	79	
1	B	79	
1	C	79	
1	D	79	
1	E	79	

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

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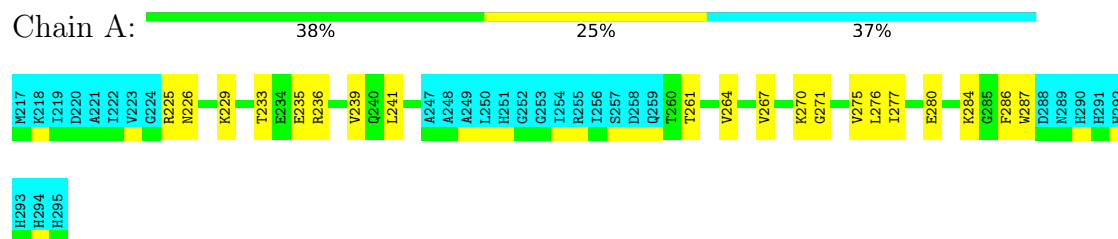
Chain	Residue	Modelled	Actual	Comment	Reference
D	291	HIS	-	expression tag	UNP Q03689
D	292	HIS	-	expression tag	UNP Q03689
D	293	HIS	-	expression tag	UNP Q03689
D	294	HIS	-	expression tag	UNP Q03689
D	295	HIS	-	expression tag	UNP Q03689
E	217	MET	-	initiating methionine	UNP Q03689
E	290	HIS	-	expression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

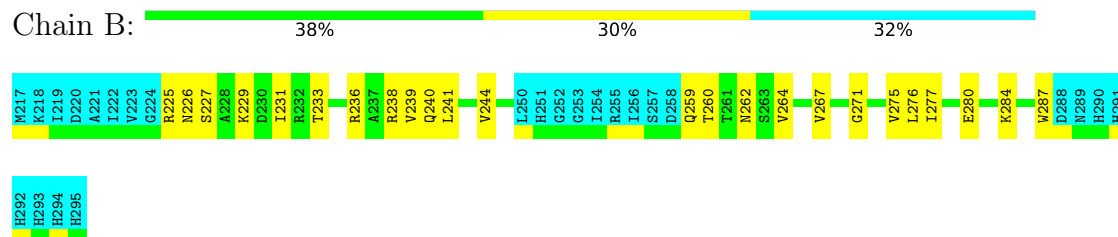
4.1 Average score per residue in the NMR ensemble

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

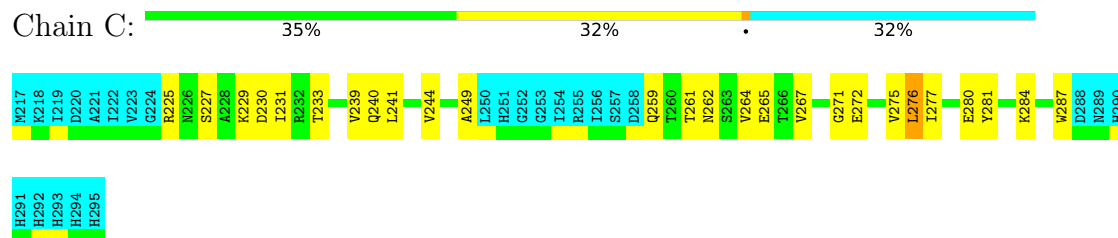
- Molecule 1: Small s protein



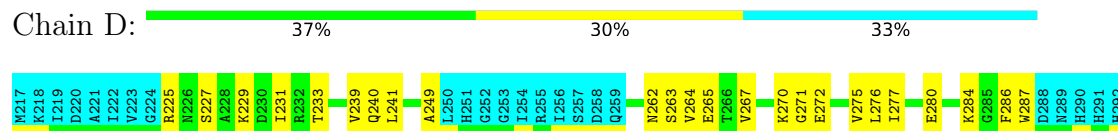
- Molecule 1: Small s protein



- Molecule 1: Small s protein

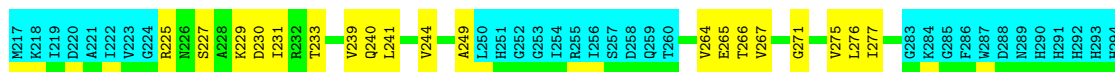


- Molecule 1: Small s protein





- Molecule 1: Small s protein

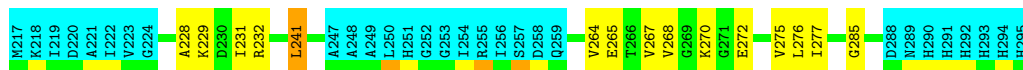


4.2 Scores per residue for each member of the ensemble

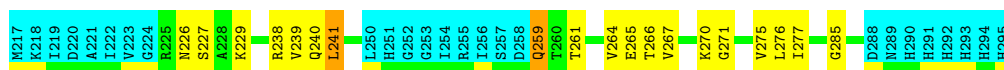
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

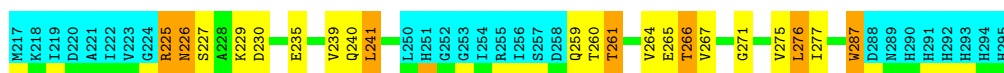
- Molecule 1: Small s protein



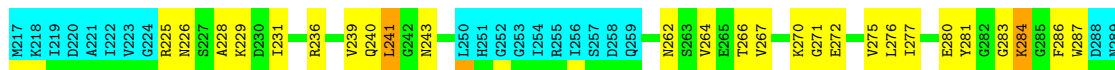
- Molecule 1: Small s protein

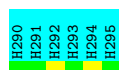


- Molecule 1: Small s protein



- Molecule 1: Small s protein





- Molecule 1: Small s protein



4.2.2 Score per residue for model 2

- Molecule 1: Small s protein



- Molecule 1: Small s protein



- Molecule 1: Small s protein

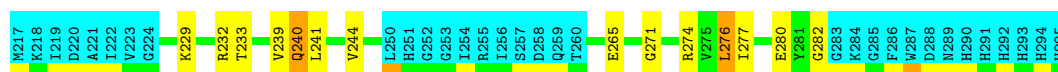


- Molecule 1: Small s protein



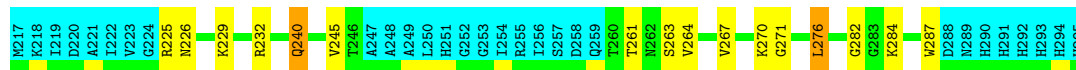
- Molecule 1: Small s protein



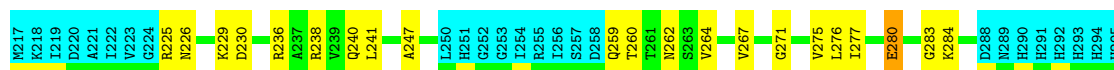


4.2.3 Score per residue for model 3

- Molecule 1: Small s protein



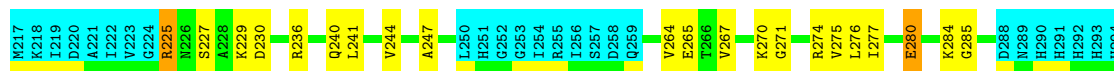
- Molecule 1: Small s protein



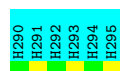
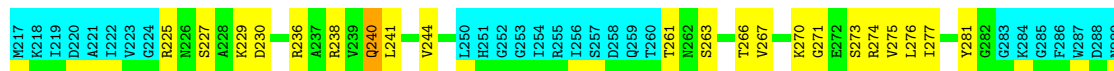
- Molecule 1: Small s protein



- Molecule 1: Small s protein

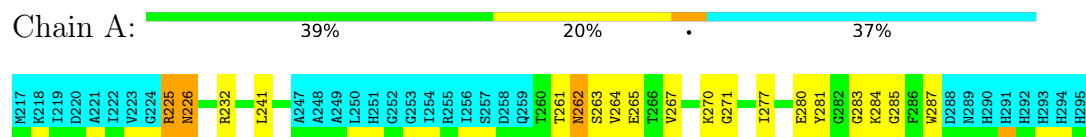


- Molecule 1: Small s protein

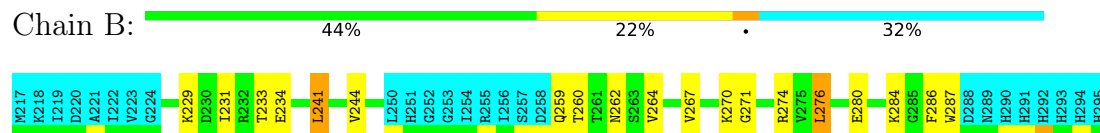


4.2.4 Score per residue for model 4

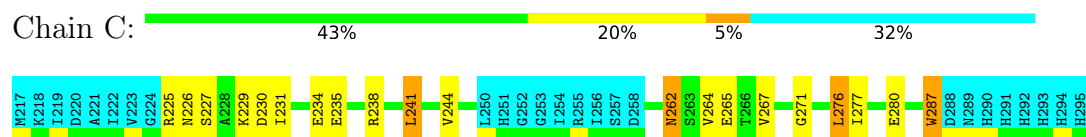
- Molecule 1: Small s protein



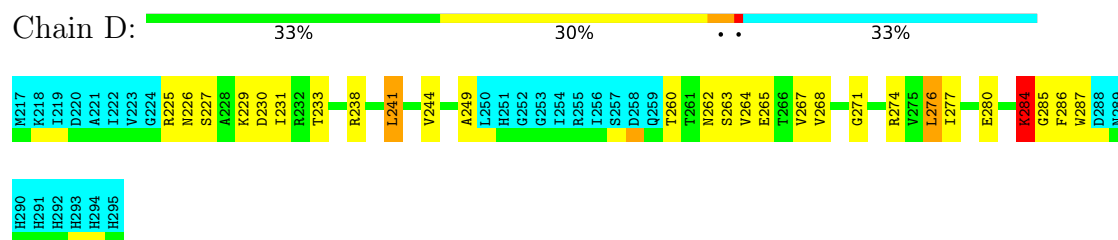
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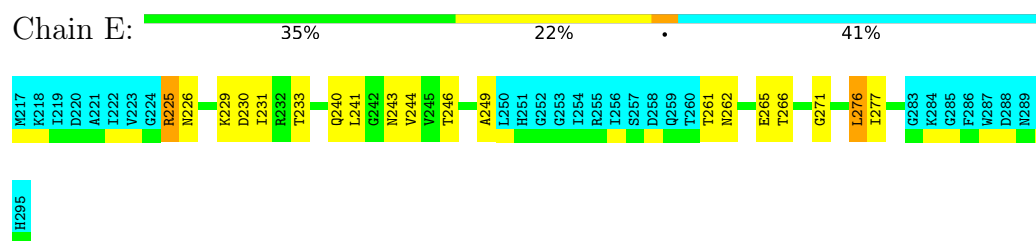
- Molecule 1: Small s protein



- Molecule 1: Small s protein

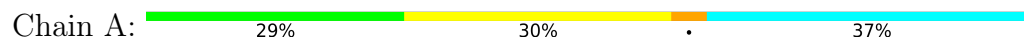


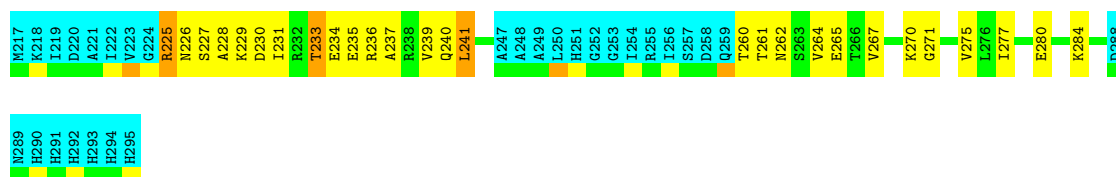
- Molecule 1: Small s protein



4.2.5 Score per residue for model 5

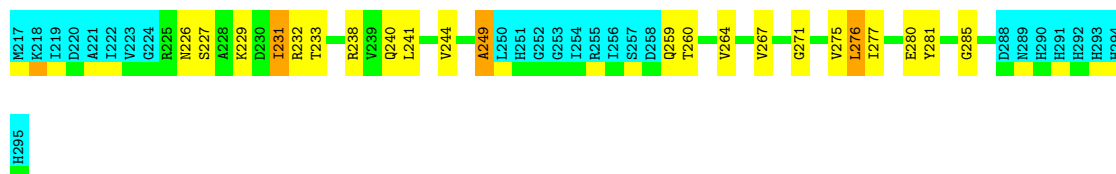
- Molecule 1: Small s protein





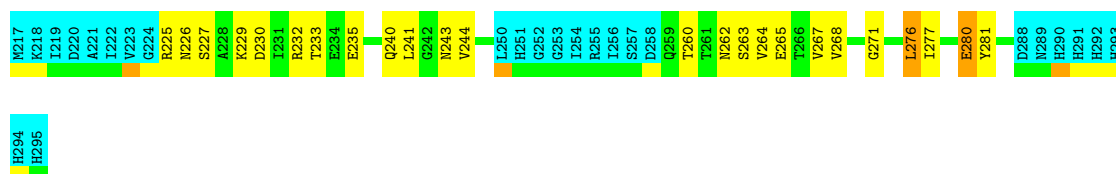
- Molecule 1: Small s protein

Chain B: 41% 24% 32%



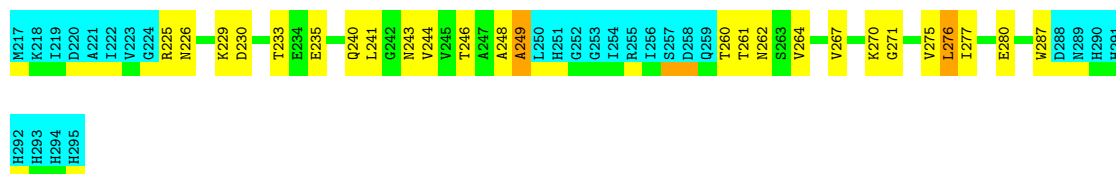
- Molecule 1: Small s protein

Chain C: 38% 28% 32%



- Molecule 1: Small s protein

Chain D: 35% 29% 33%



- Molecule 1: Small s protein

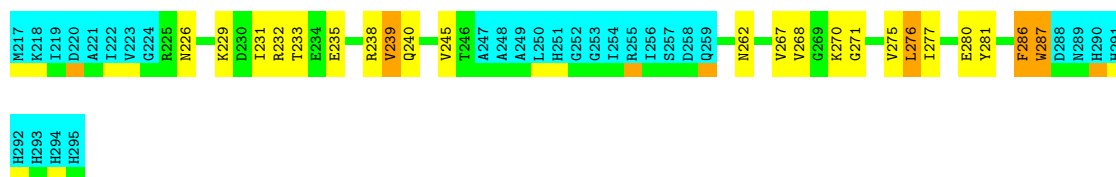
Chain E: 39% 18% 41%



4.2.6 Score per residue for model 6

- Molecule 1: Small s protein

Chain A: 35% 23% 5% 37%



- Molecule 1: Small s protein

Chain B: 33% 28% 8% 32%



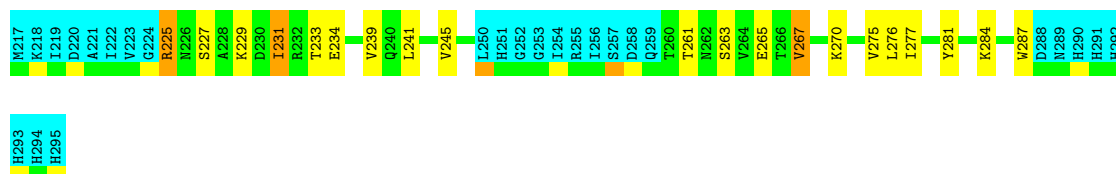
- Molecule 1: Small s protein

Chain C: 39% 23% 6% 32%



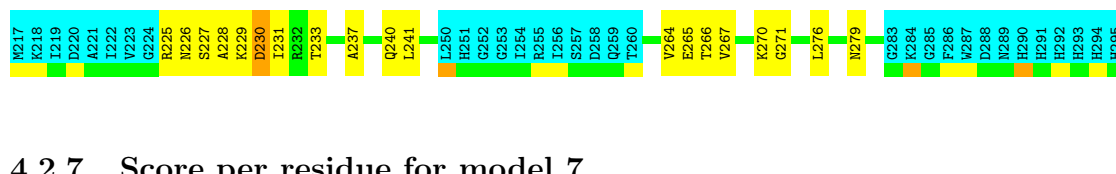
- Molecule 1: Small s protein

Chain D: 42% 22% 0% 33%



- Molecule 1: Small s protein

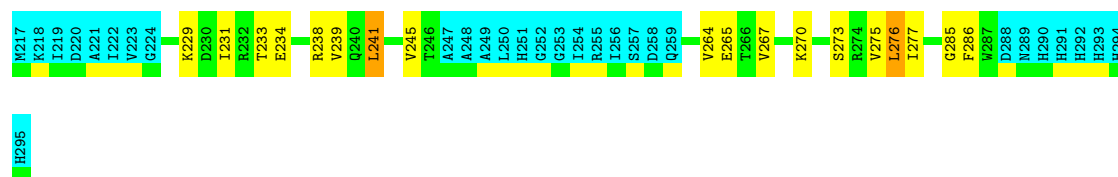
Chain E: 35% 23% 0% 41%



4.2.7 Score per residue for model 7

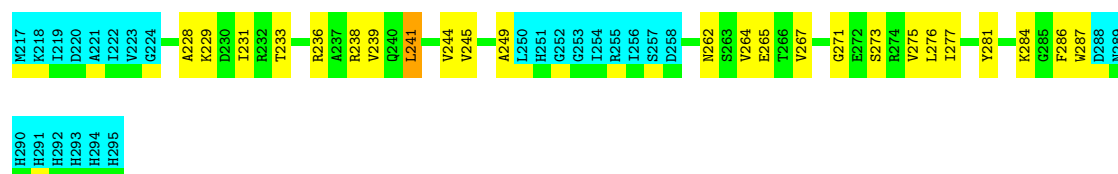
- Molecule 1: Small s protein

Chain A: 41% 20% 0% 37%



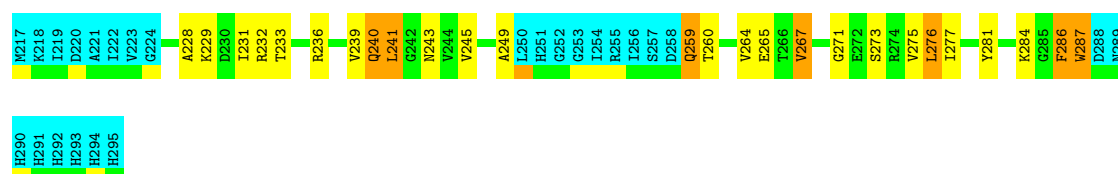
- Molecule 1: Small s protein

Chain B: 38% 29% 32%



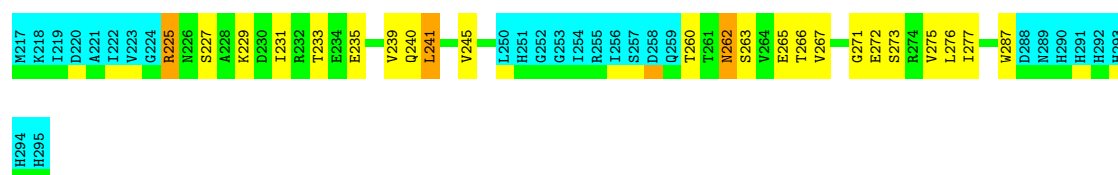
- Molecule 1: Small s protein

Chain C: 35% 24% 9% 32%



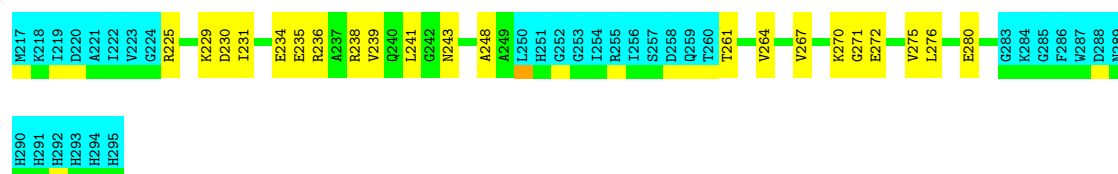
- Molecule 1: Small s protein

Chain D: 38% 25% 33%



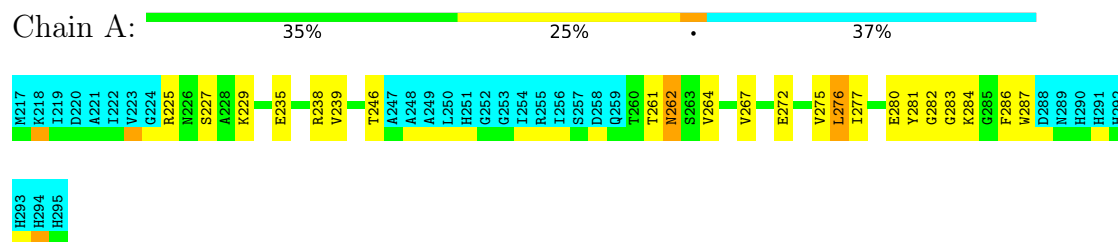
- Molecule 1: Small s protein

Chain E: 33% 27% 41%

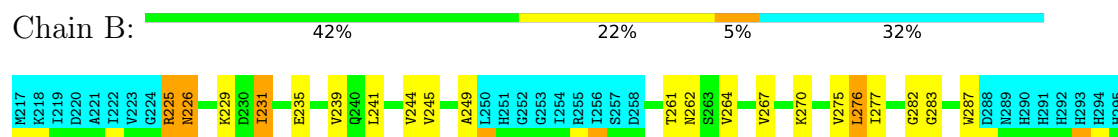


4.2.8 Score per residue for model 8

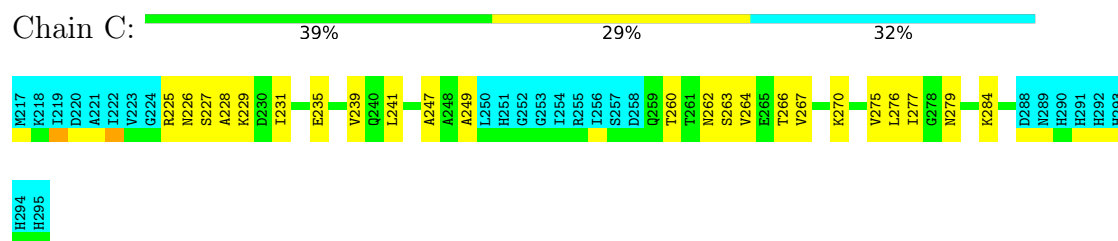
- Molecule 1: Small s protein



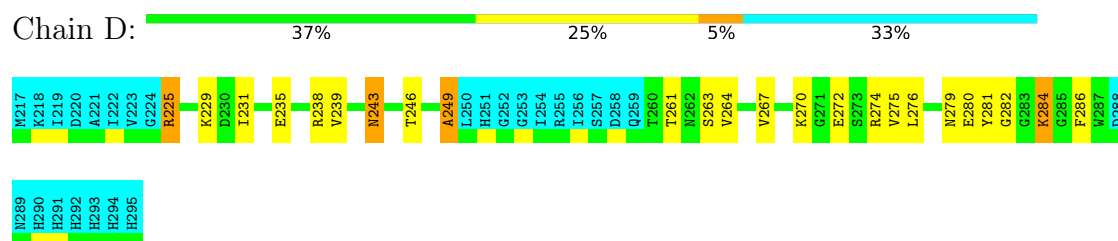
- Molecule 1: Small s protein



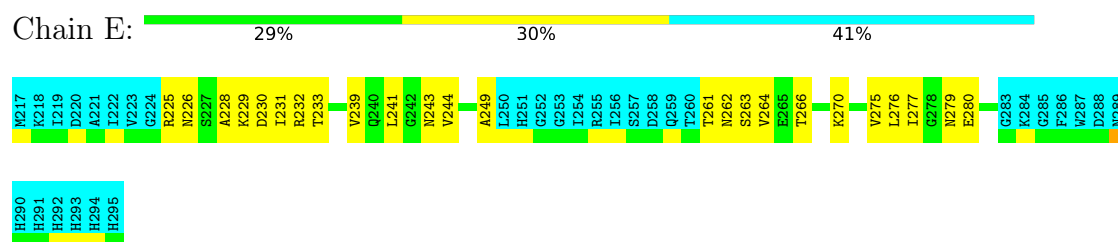
- Molecule 1: Small s protein



- Molecule 1: Small s protein

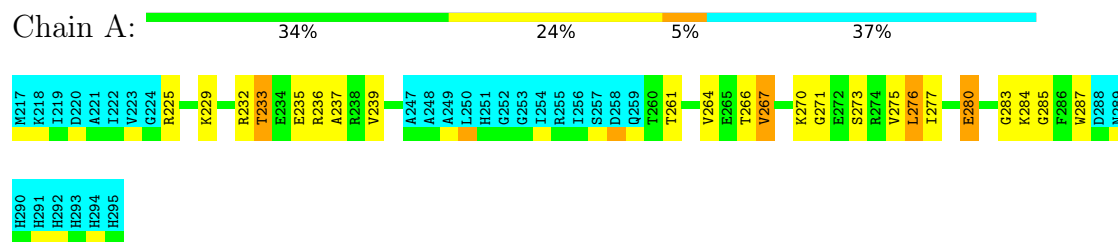


- Molecule 1: Small s protein

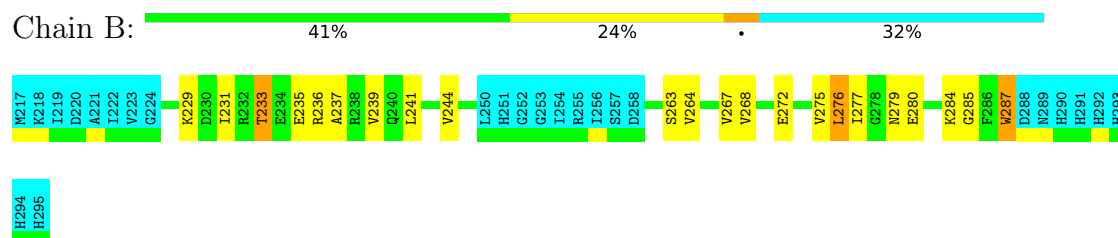


4.2.9 Score per residue for model 9

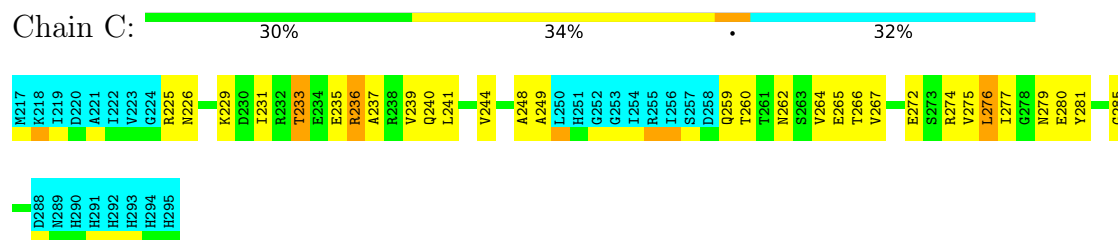
- Molecule 1: Small s protein



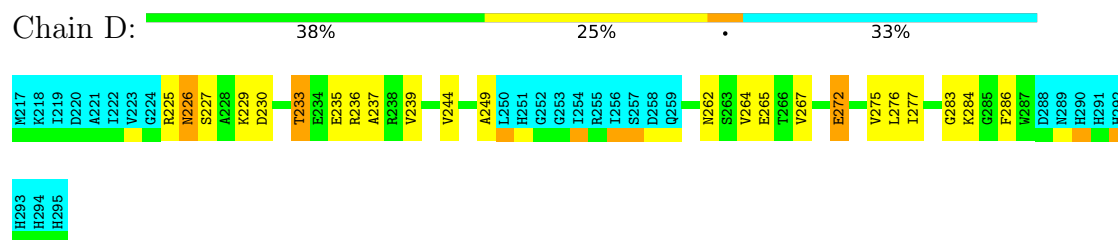
- Molecule 1: Small s protein



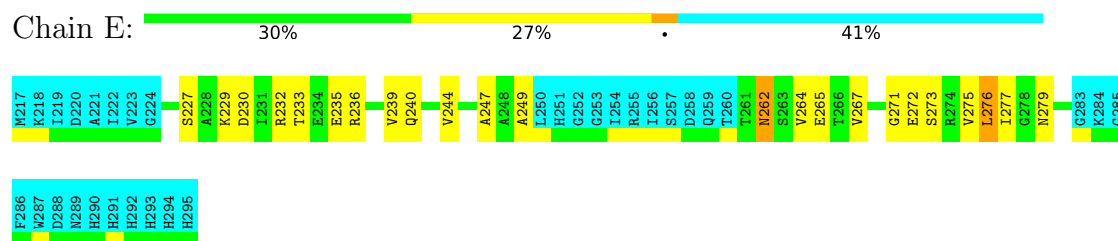
- Molecule 1: Small s protein



- Molecule 1: Small s protein

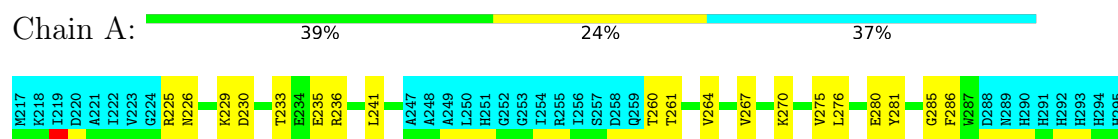


- Molecule 1: Small s protein

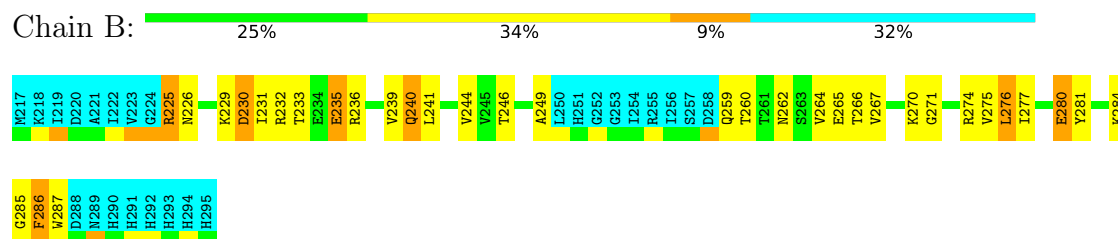


4.2.10 Score per residue for model 10

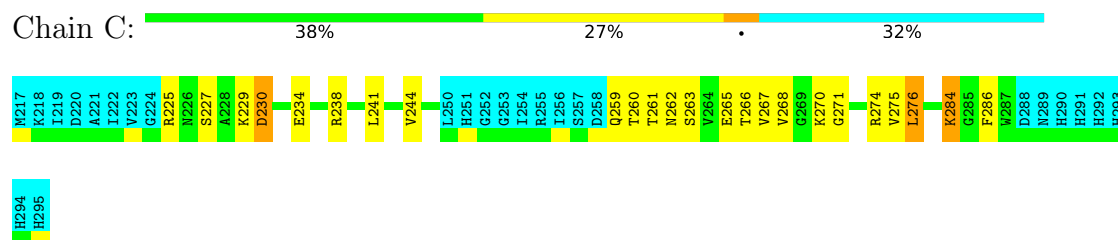
- Molecule 1: Small s protein



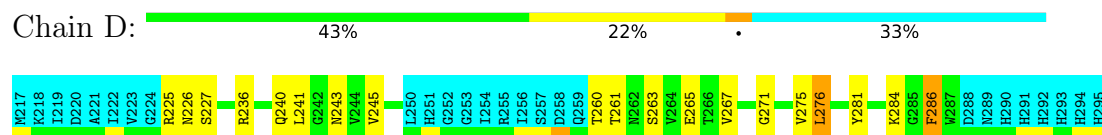
- Molecule 1: Small s protein



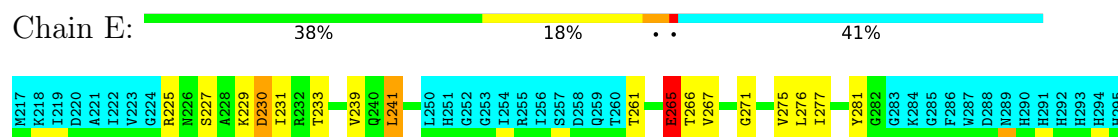
- Molecule 1: Small s protein



- Molecule 1: Small s protein



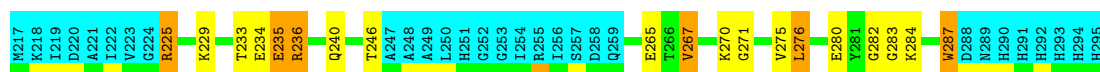
- Molecule 1: Small s protein



4.2.11 Score per residue for model 11

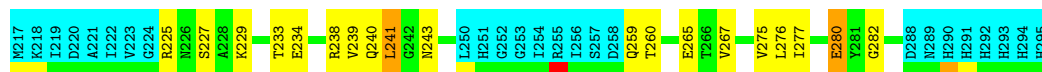
- Molecule 1: Small s protein





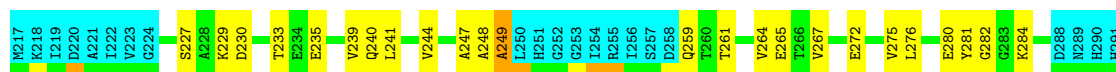
- Molecule 1: Small s protein

Chain B: 44% 22% 32%



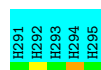
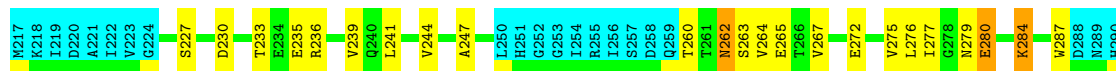
- Molecule 1: Small s protein

Chain C: 38% 29% 32%



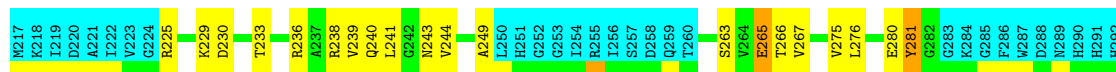
- Molecule 1: Small s protein

Chain D: 38% 25% 33%



- Molecule 1: Small s protein

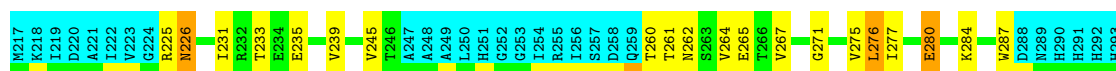
Chain E: 34% 23% 41%



4.2.12 Score per residue for model 12

- Molecule 1: Small s protein

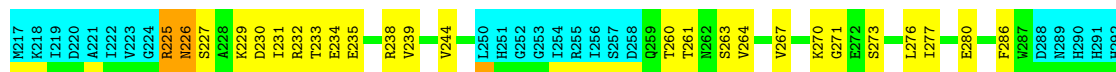
Chain A: 38% 22% 37%





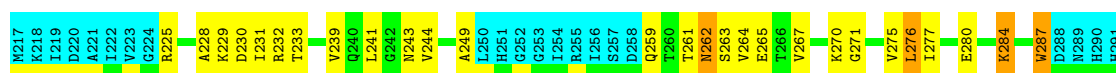
- Molecule 1: Small s protein

Chain B: 37% 29% 32%



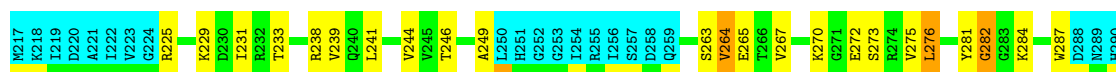
- Molecule 1: Small s protein

Chain C: 34% 29% 5% 32%



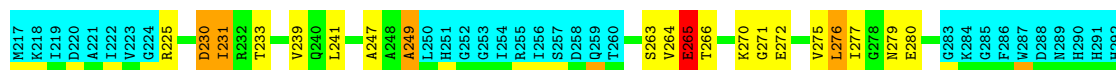
- Molecule 1: Small s protein

Chain D: 38% 25% 33%



- Molecule 1: Small s protein

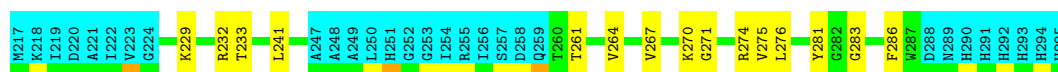
Chain E: 34% 19% 5% 41%



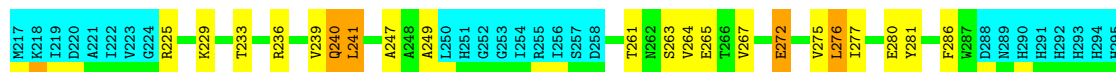
4.2.13 Score per residue for model 13

- Molecule 1: Small s protein

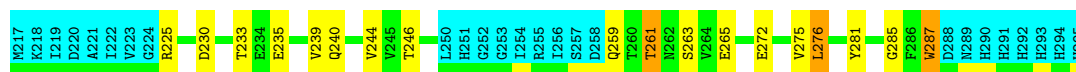
Chain A: 44% 19% 37%



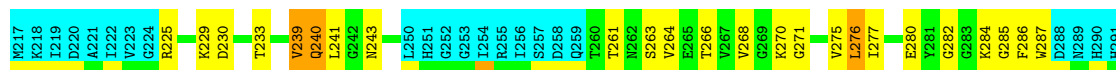
- Molecule 1: Small s protein



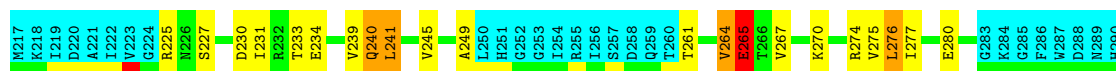
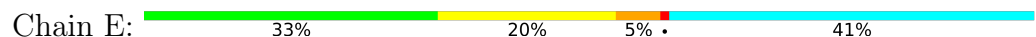
- Molecule 1: Small s protein



- Molecule 1: Small s protein



- Molecule 1: Small s protein



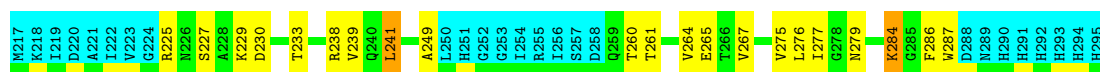
4.2.14 Score per residue for model 14

- Molecule 1: Small s protein



- Molecule 1: Small s protein

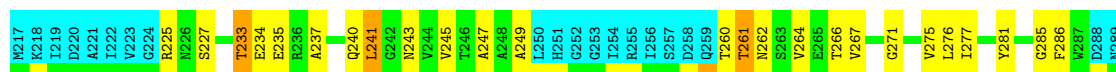




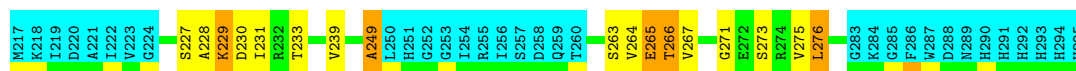
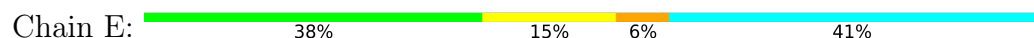
- Molecule 1: Small s protein



- Molecule 1: Small s protein

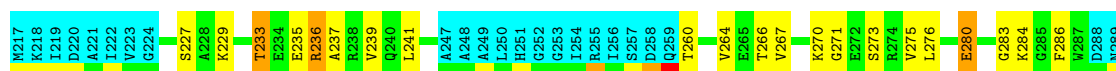


- Molecule 1: Small s protein

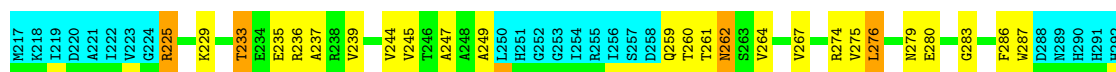


4.2.15 Score per residue for model 15

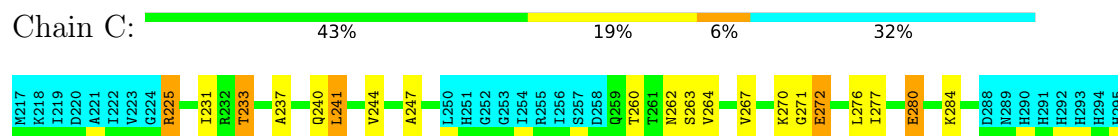
- Molecule 1: Small s protein



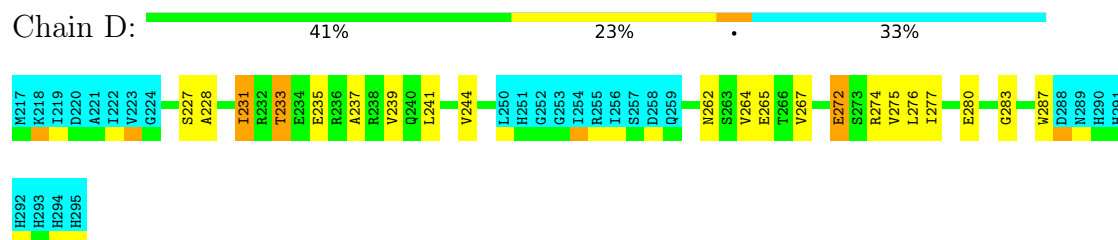
- Molecule 1: Small s protein



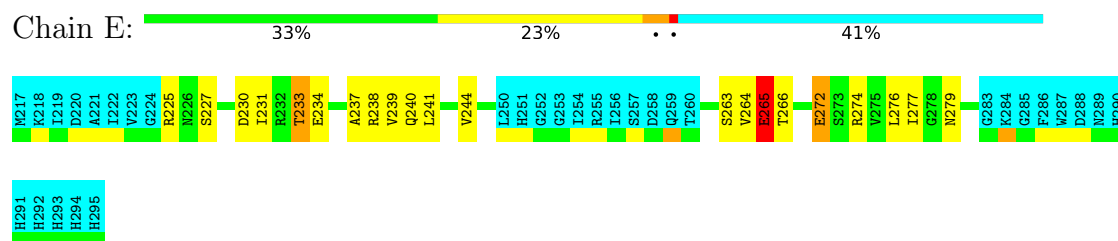
- Molecule 1: Small s protein



- Molecule 1: Small s protein

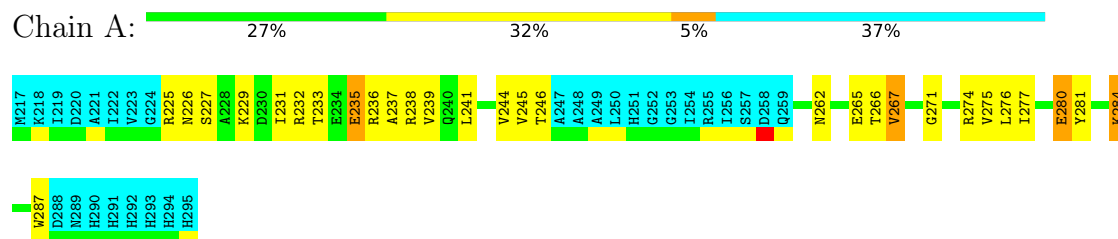


- Molecule 1: Small s protein

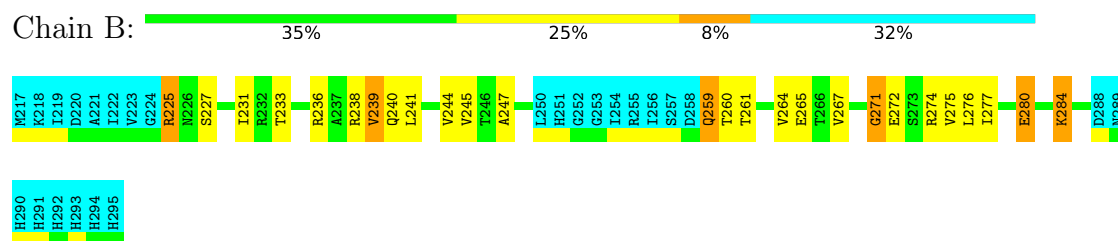


4.2.16 Score per residue for model 16

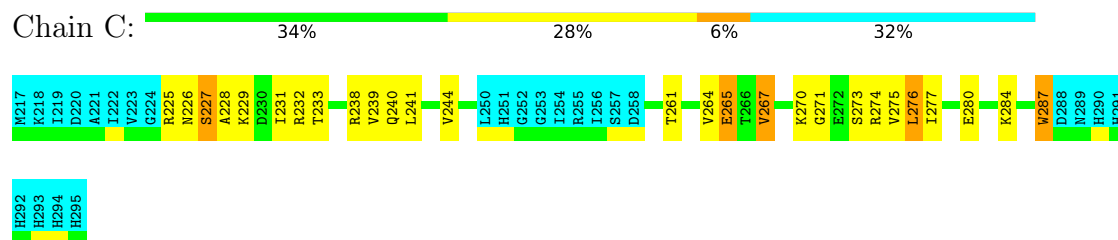
- Molecule 1: Small s protein



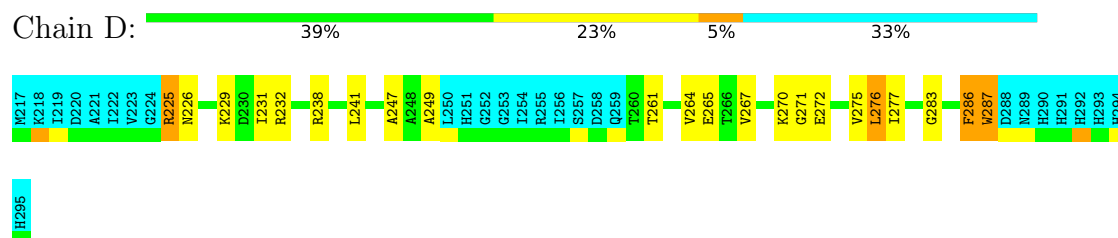
- Molecule 1: Small s protein



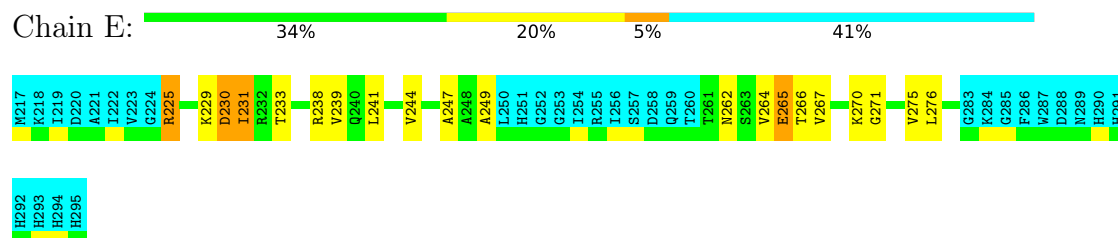
- Molecule 1: Small s protein



- Molecule 1: Small s protein

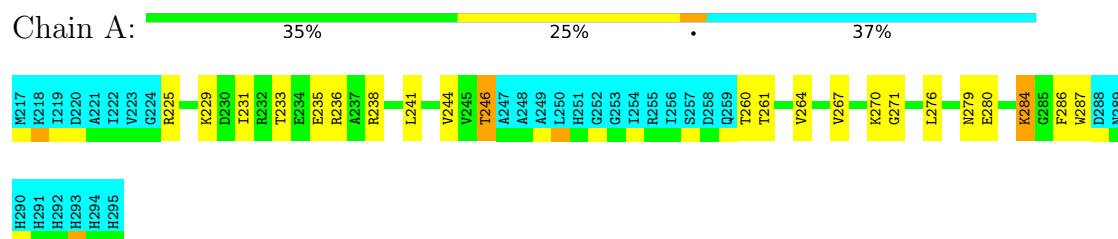


- Molecule 1: Small s protein

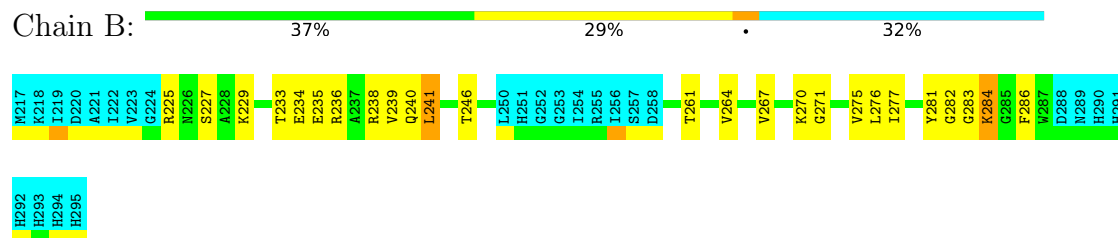


4.2.17 Score per residue for model 17

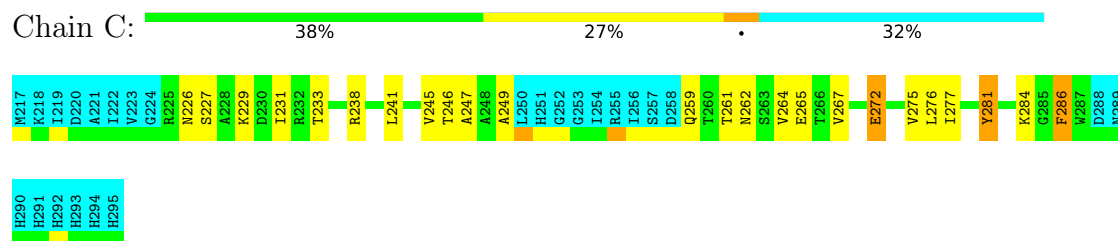
- Molecule 1: Small s protein



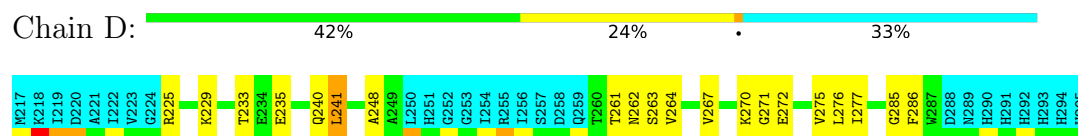
- Molecule 1: Small s protein



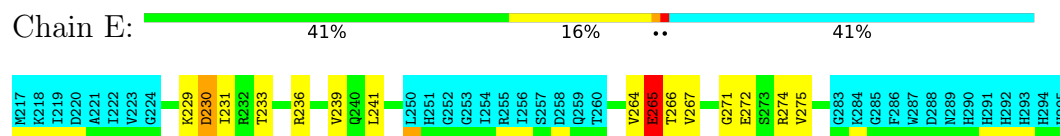
- Molecule 1: Small s protein



- Molecule 1: Small s protein

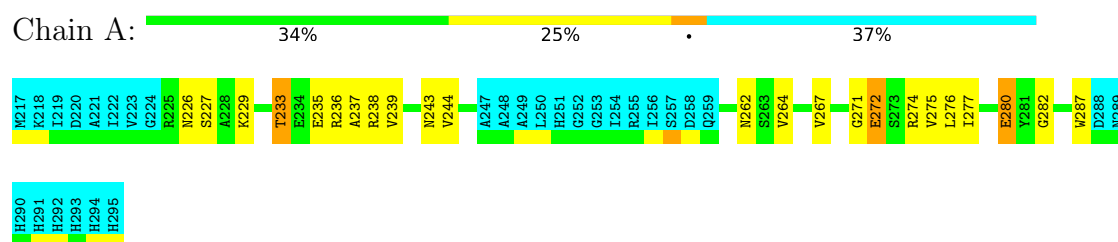


- Molecule 1: Small s protein

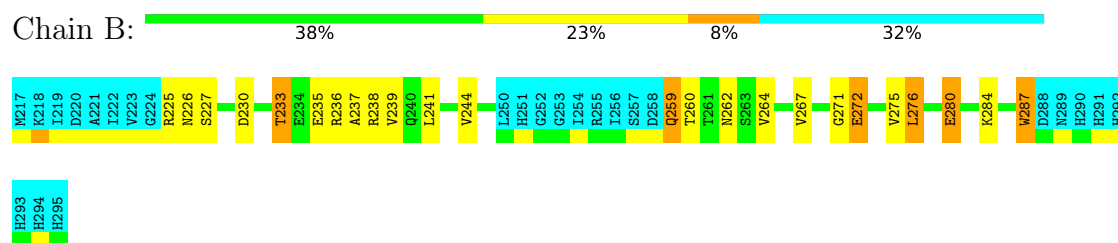


4.2.18 Score per residue for model 18

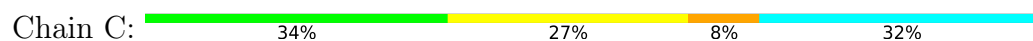
- Molecule 1: Small s protein

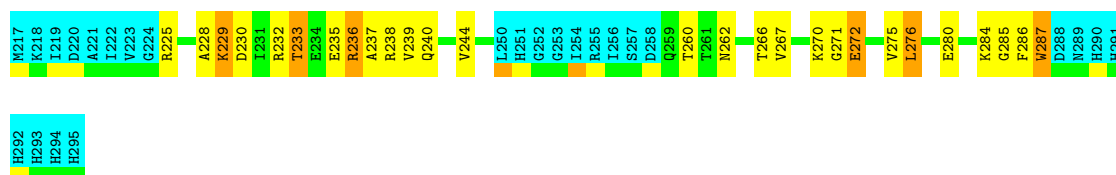


- Molecule 1: Small s protein

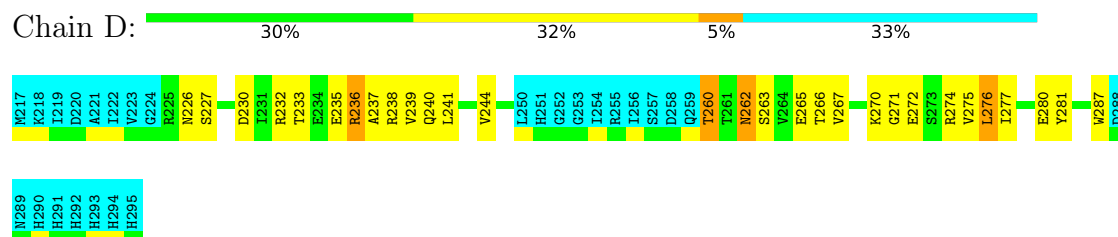


- Molecule 1: Small s protein

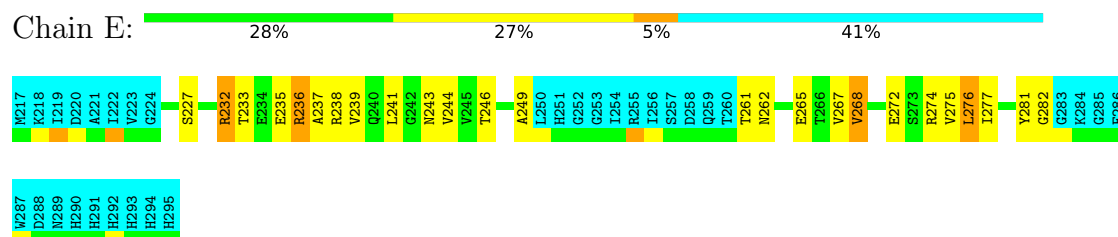




- Molecule 1: Small s protein

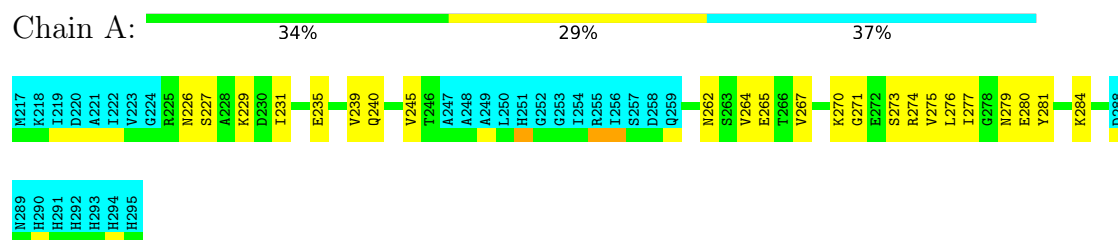


- Molecule 1: Small s protein

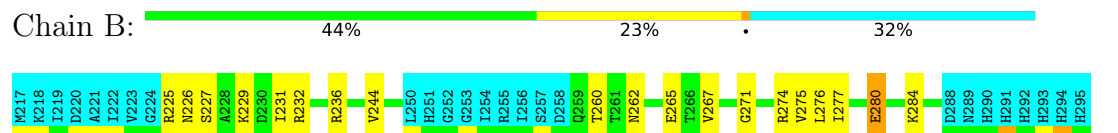


4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: Small s protein

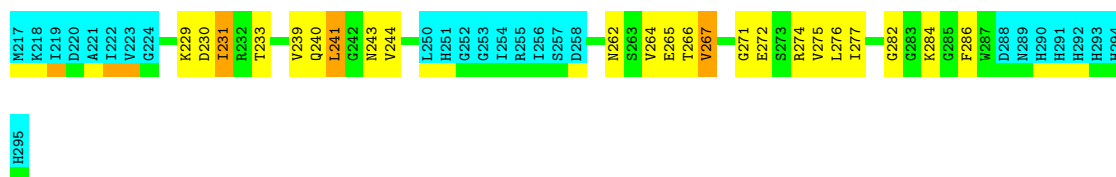


- Molecule 1: Small s protein



- Molecule 1: Small s protein





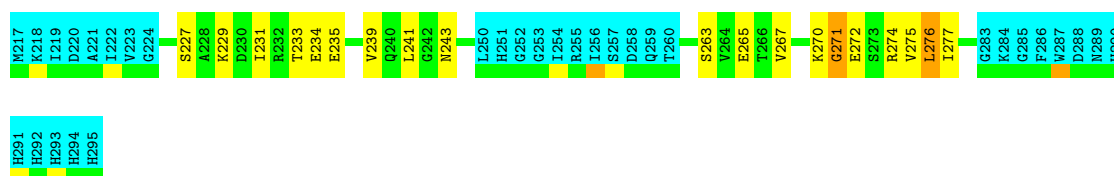
- Molecule 1: Small s protein

Chain D: 41% 20% 6% 33%



- Molecule 1: Small s protein

Chain E: 35% 22% 0% 41%



4.2.20 Score per residue for model 20

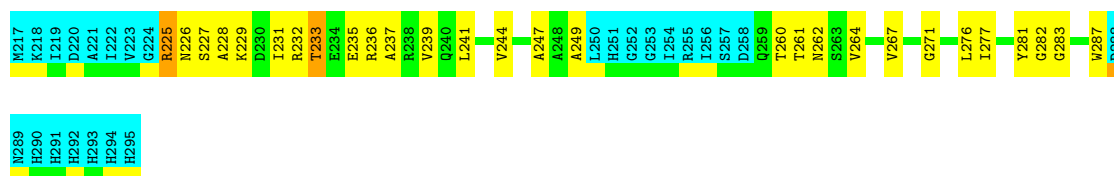
- Molecule 1: Small s protein

Chain A: 37% 22% 5% 37%



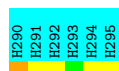
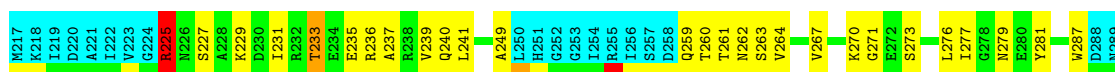
- Molecule 1: Small s protein

Chain B: 33% 33% 0% 32%



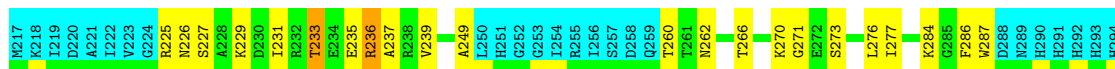
- Molecule 1: Small s protein

Chain C: 34% 32% 0% 32%



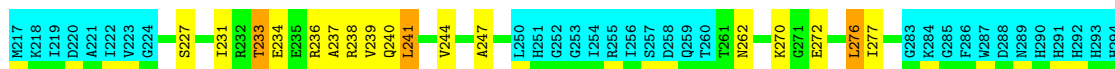
- Molecule 1: Small s protein

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	10±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	10±3
All	All	39080	39220	39220	929

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

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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:260:THR:HG21	1:E:243:ASN:CG	0.66	2.16	4	1
1:C:240:GLN:C	1:C:241:LEU:HD13	0.66	2.16	1	3
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:B:240:GLN:C	1:B:241:LEU:HD13	0.65	2.16	1	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:D:240:GLN:C	1:D:241:LEU:HD13	0.62	2.18	1	3
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:E:265:GLU:N	1:E:265:GLU:CD	0.62	2.58	12	4
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:E:231:ILE:HG21	1:E:239:VAL:HG21	0.61	1.72	19	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:E:231:ILE:HG23	1:E:267:VAL:CG2	0.60	2.27	6	1
1:A:280:GLU:CD	1:B:244:VAL:HG13	0.60	2.22	15	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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: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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:280:GLU:CG	1:B:244:VAL:HG23	0.56	2.31	5	1
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:D:280:GLU:CD	1:E:244:VAL:HG13	0.55	2.27	11	2
1:C:240:GLN:C	1:C:241:LEU:HD22	0.55	2.27	5	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:B:280:GLU:CD	1:C:244:VAL:HG13	0.53	2.28	3	2
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:A:235:GLU:O	1:A:236:ARG:C	0.52	2.52	2	6
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:E:235:GLU:O	1:E:236:ARG:C	0.51	2.52	7	1
1:A:232:ARG:HD2	1:A:268:VAL:HG22	0.51	1.81	1	1
1:D:264:VAL:HG21	1:D:277:ILE:CD1	0.51	2.35	9	1
1:E:240:GLN:C	1:E:241:LEU:HD13	0.51	2.31	20	2
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: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: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:260:THR:HG21	1:D:243:ASN:CG	0.50	2.31	10	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:E:246:THR:HG21	1:E:282:GLY:C	0.50	2.32	18	1
1:D:264:VAL:HG21	1:D:267:VAL:CG2	0.50	2.37	14	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:E:229:LYS:HE2	1:E:265:GLU:C	0.49	2.32	14	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:E:265:GLU:CD	1:E:265:GLU:C	0.49	2.80	13	5
1:D:275:VAL:C	1:D:276:LEU:HD23	0.49	2.33	6	1
1:D:276:LEU:HD12	1:D:287:TRP:CD2	0.49	2.43	16	1
1:B:240:GLN:C	1:B:241:LEU:HD23	0.49	2.33	17	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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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
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:240:GLN:C	1:D:241:LEU:HD22	0.47	2.35	19	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: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: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:E:265:GLU:CD	1:E:265:GLU:N	0.46	2.73	13	1
1:B:262:ASN:OD1	1:C:241:LEU:HD12	0.46	2.10	6	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: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:235:GLU:O	1:B:236:ARG:C	0.46	2.57	10	2
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
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: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: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:C:260:THR:HG21	1:C:279:ASN:CG	0.45	2.37	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:E:240:GLN:C	1:E:241:LEU:HD12	0.45	2.37	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
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: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: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:B:276:LEU:C	1:B:276:LEU:HD13	0.44	2.38	14	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:240:GLN:C	1:E:241:LEU:HD22	0.43	2.38	2	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
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:C:280:GLU:CD	1:D:244:VAL:HG13	0.42	2.39	18	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:B:271:GLY:O	1:B:272:GLU:C	0.42	2.63	6	2
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:D:280:GLU:OE2	1:E:244:VAL:HG13	0.41	2.15	3	1
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:C:280:GLU:CD	1:D:244:VAL:HG22	0.41	2.40	11	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:276:LEU:C	1:E:276:LEU:HD13	0.41	2.41	5	1
1:A:286:PHE:O	1:A:287:TRP:C	0.41	2.62	6	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:271:GLY:O	1:C:272:GLU:C	0.40	2.63	6	1
1:E:271:GLY:O	1:E:272:GLU:C	0.40	2.64	19	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%)	3	27
1	B	54/79 (68%)	45±2 (84±4%)	6±2 (12±3%)	2±1 (4±2%)	4	30
1	C	54/79 (68%)	46±2 (84±3%)	6±2 (11±3%)	3±1 (5±2%)	3	24
1	D	53/79 (67%)	44±2 (84±3%)	6±2 (11±3%)	3±1 (5±2%)	2	21
1	E	47/79 (59%)	41±1 (87±2%)	4±1 (9±3%)	2±1 (5±2%)	3	26
All	All	5160/7900 (65%)	4362 (85%)	556 (11%)	242 (5%)	3	25

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

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Mol	Chain	Res	Type	Models (Total)
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
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

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Mol	Chain	Res	Type	Models (Total)
1	B	283	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	41/63 (65%)	30±2 (74±6%)	10±2 (26±6%)	2	23
1	B	42/63 (67%)	31±2 (73±5%)	11±2 (27±5%)	2	22
1	C	42/63 (67%)	31±2 (73±5%)	11±2 (27±5%)	2	22
1	D	41/63 (65%)	30±2 (73±6%)	11±2 (27±6%)	1	21
1	E	37/63 (59%)	27±3 (73±7%)	10±3 (27±7%)	2	21
All	All	4060/6300 (64%)	2981 (73%)	1079 (27%)	2	22

All 179 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	20
1	A	229	LYS	18
1	B	276	LEU	18
1	C	229	LYS	18
1	A	276	LEU	17
1	B	229	LYS	17
1	D	276	LEU	16
1	E	276	LEU	16
1	C	265	GLU	15
1	E	229	LYS	15
1	A	270	LYS	14
1	D	229	LYS	13
1	D	270	LYS	13
1	B	233	THR	13
1	E	265	GLU	13
1	B	227	SER	12
1	D	262	ASN	12
1	A	233	THR	12
1	E	233	THR	12

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Mol	Chain	Res	Type	Models (Total)
1	A	284	LYS	12
1	E	230	ASP	12
1	B	238	ARG	11
1	C	233	THR	11
1	D	265	GLU	11
1	B	284	LYS	11
1	D	227	SER	11
1	E	227	SER	11
1	A	241	LEU	10
1	A	265	GLU	10
1	B	241	LEU	10
1	B	265	GLU	10
1	C	225	ARG	10
1	D	225	ARG	10
1	D	284	LYS	10
1	E	270	LYS	10
1	D	233	THR	10
1	B	225	ARG	10
1	D	263	SER	10
1	A	235	GLU	10
1	C	235	GLU	9
1	C	241	LEU	9
1	C	259	GLN	9
1	C	262	ASN	9
1	D	235	GLU	9
1	C	227	SER	8
1	D	241	LEU	8
1	E	263	SER	8
1	E	274	ARG	8
1	A	227	SER	8
1	C	230	ASP	8
1	C	263	SER	8
1	C	284	LYS	8
1	B	235	GLU	8
1	B	270	LYS	7
1	D	236	ARG	7
1	D	272	GLU	7
1	E	225	ARG	7
1	E	280	GLU	7
1	D	230	ASP	7
1	E	238	ARG	7
1	A	238	ARG	7

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Mol	Chain	Res	Type	Models (Total)
1	C	270	LYS	7
1	A	280	GLU	7
1	C	226	ASN	6
1	D	266	THR	6
1	A	225	ARG	6
1	B	226	ASN	6
1	B	230	ASP	6
1	D	226	ASN	6
1	B	236	ARG	6
1	B	240	GLN	6
1	B	280	GLU	6
1	D	274	ARG	6
1	A	262	ASN	6
1	B	259	GLN	6
1	B	262	ASN	6
1	B	274	ARG	6
1	E	262	ASN	6
1	E	234	GLU	6
1	C	240	GLN	6
1	A	236	ARG	5
1	A	274	ARG	5
1	D	240	GLN	5
1	E	240	GLN	5
1	A	226	ASN	5
1	A	232	ARG	5
1	A	240	GLN	5
1	C	232	ARG	5
1	C	274	ARG	5
1	C	280	GLU	5
1	D	280	GLU	5
1	C	238	ARG	5
1	D	238	ARG	5
1	A	260	THR	5
1	B	232	ARG	5
1	E	261	THR	5
1	E	266	THR	5
1	A	273	SER	5
1	E	241	LEU	5
1	A	286	PHE	4
1	B	281	TYR	4
1	C	234	GLU	4
1	E	232	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	E	236	ARG	4
1	B	234	GLU	4
1	B	286	PHE	4
1	E	226	ASN	4
1	C	267	VAL	4
1	C	260	THR	4
1	E	243	ASN	4
1	A	246	THR	4
1	D	243	ASN	4
1	A	261	THR	4
1	C	286	PHE	4
1	B	260	THR	4
1	D	260	THR	4
1	C	272	GLU	4
1	A	272	GLU	3
1	C	261	THR	3
1	C	266	THR	3
1	A	263	SER	3
1	E	273	SER	3
1	E	281	TYR	3
1	A	281	TYR	3
1	A	234	GLU	3
1	E	272	GLU	3
1	B	273	SER	3
1	B	287	TRP	3
1	D	231	ILE	3
1	D	261	THR	3
1	D	267	VAL	3
1	D	287	TRP	3
1	C	236	ARG	3
1	C	273	SER	3
1	D	273	SER	3
1	E	231	ILE	3
1	E	279	ASN	3
1	A	266	THR	3
1	A	267	VAL	3
1	B	263	SER	3
1	B	279	ASN	3
1	E	235	GLU	3
1	D	286	PHE	3
1	B	243	ASN	2
1	D	268	VAL	2

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Mol	Chain	Res	Type	Models (Total)
1	A	230	ASP	2
1	B	231	ILE	2
1	B	239	VAL	2
1	C	281	TYR	2
1	D	234	GLU	2
1	C	279	ASN	2
1	D	279	ASN	2
1	E	244	VAL	2
1	E	264	VAL	2
1	C	231	ILE	2
1	B	272	GLU	2
1	D	232	ARG	2
1	A	244	VAL	2
1	B	266	THR	1
1	B	246	THR	1
1	C	243	ASN	1
1	A	239	VAL	1
1	C	239	VAL	1
1	B	267	VAL	1
1	B	268	VAL	1
1	C	268	VAL	1
1	D	244	VAL	1
1	D	264	VAL	1
1	B	261	THR	1
1	D	239	VAL	1
1	E	245	VAL	1
1	B	245	VAL	1
1	A	231	ILE	1
1	A	243	ASN	1
1	C	287	TRP	1
1	E	268	VAL	1
1	A	279	ASN	1
1	D	277	ILE	1
1	B	244	VAL	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 [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