



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:19 PM BST

PDB ID : 1DV9
Title : STRUCTURAL CHANGES ACCOMPANYING PH-INDUCED DISSOCIATION OF THE B-LACTOGLOBULIN DIMER
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Deposited on : 2000-01-20

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

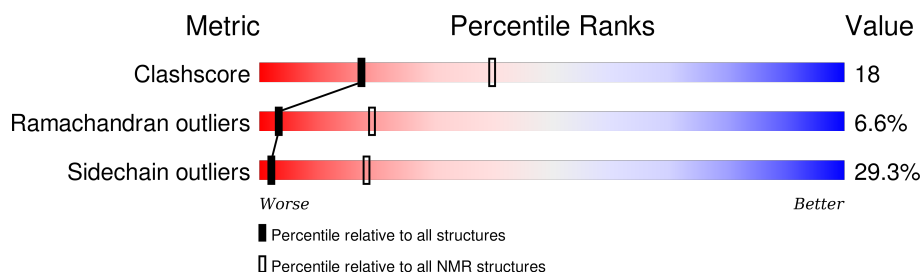
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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

Mol	Chain	Length	Quality of chain
1	A	162	

2 Ensemble composition and analysis

This entry contains 21 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 14 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:6-A:33, A:37-A:60, A:66-A:156 (143)	0.53	5

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

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

The models can be grouped into 2 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 5, 6, 7, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19
2	2, 20
Single-model clusters	8; 21

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2590 atoms, of which 1303 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BETA-LACTOGLOBULIN.

Mol	Chain	Residues	Atoms						Trace
1	A	162	Total	C	H	N	O	S	0
			2590	821	1303	206	251	9	

There are 3 discrepancies between the modelled and reference sequences:

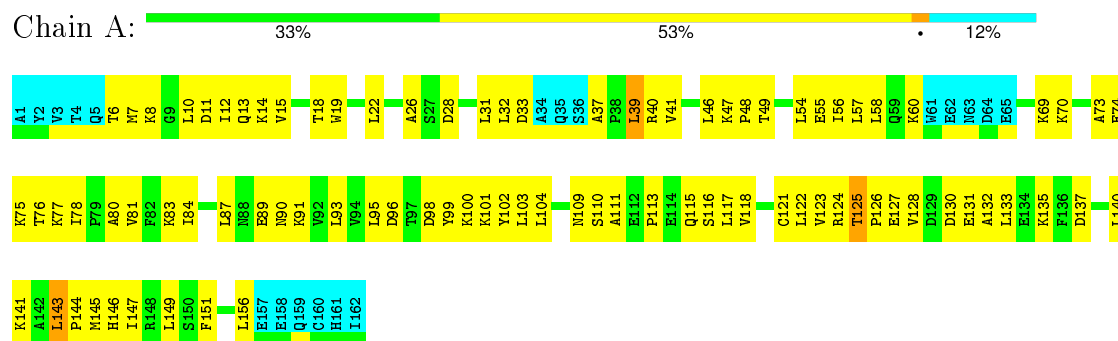
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	LEU	see remark 999	UNP P02754
A	2	TYR	ILE	see remark 999	UNP P02754
A	105	PHE	VAL	see remark 999	UNP P02754

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: BETA-LACTOGLOBULIN

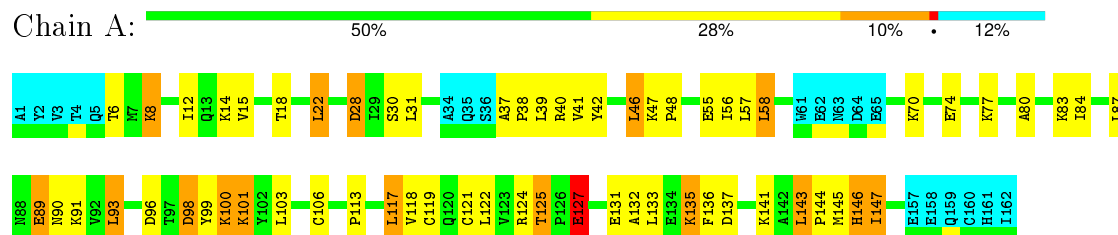


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

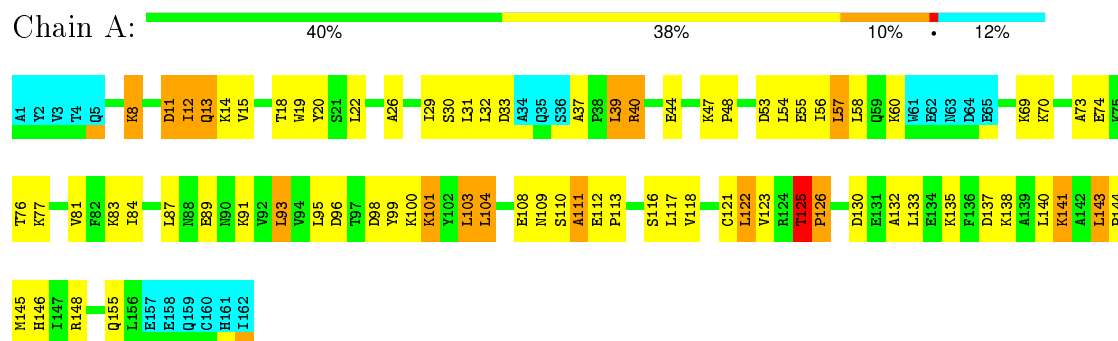
4.2.1 Score per residue for model 1

• Molecule 1: BETA-LACTOGLOBULIN



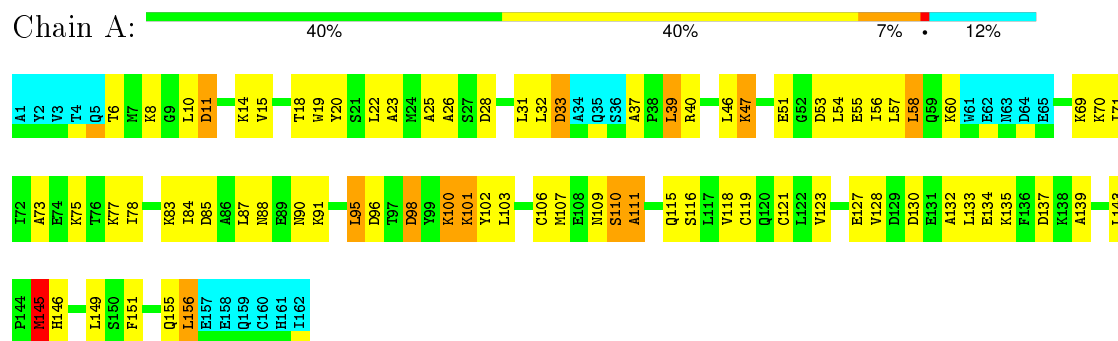
4.2.2 Score per residue for model 2

• Molecule 1: BETA-LACTOGLOBULIN



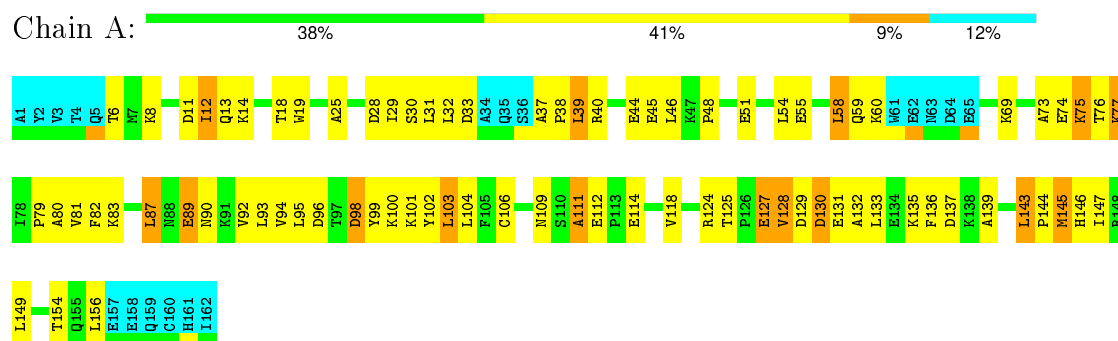
4.2.3 Score per residue for model 3

- Molecule 1: BETA-LACTOGLOBULIN



4.2.4 Score per residue for model 4

- Molecule 1: BETA-LACTOGLOBULIN



4.2.5 Score per residue for model 5 (medoid)

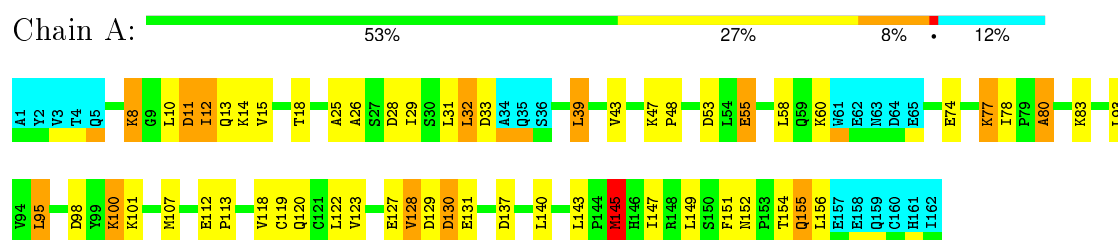
- Molecule 1: BETA-LACTOGLOBULIN





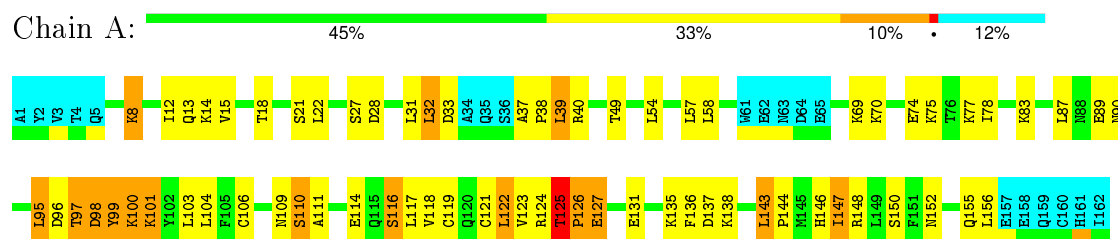
4.2.6 Score per residue for model 6

- Molecule 1: BETA-LACTOGLOBULIN



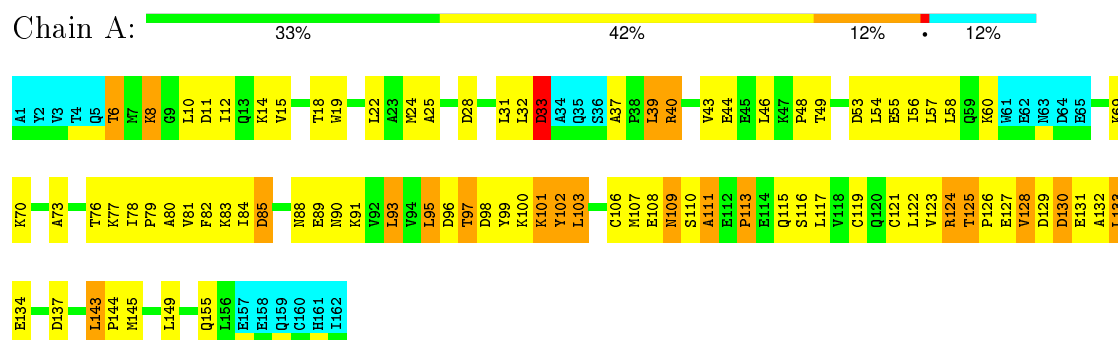
4.2.7 Score per residue for model 7

- Molecule 1: BETA-LACTOGLOBULIN



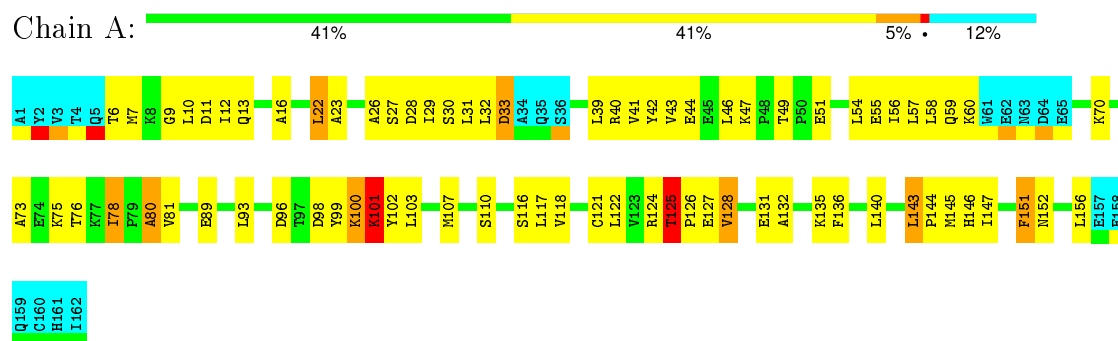
4.2.8 Score per residue for model 8

- Molecule 1: BETA-LACTOGLOBULIN



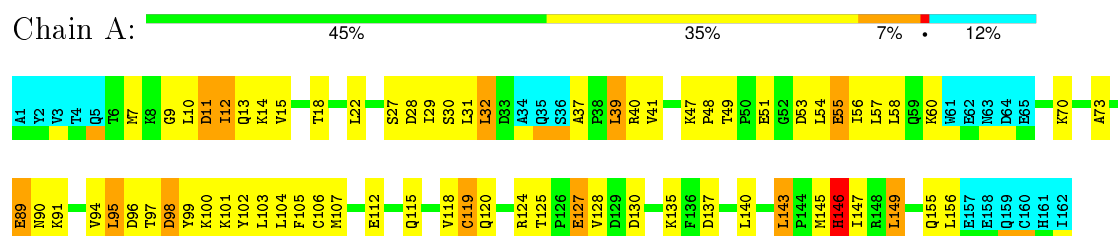
4.2.9 Score per residue for model 9

- Molecule 1: BETA-LACTOGLOBULIN



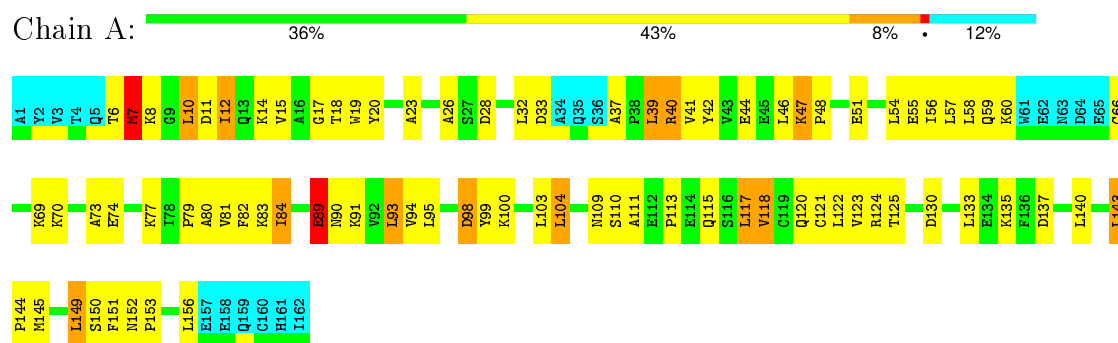
4.2.10 Score per residue for model 10

- Molecule 1: BETA-LACTOGLOBULIN



4.2.11 Score per residue for model 11

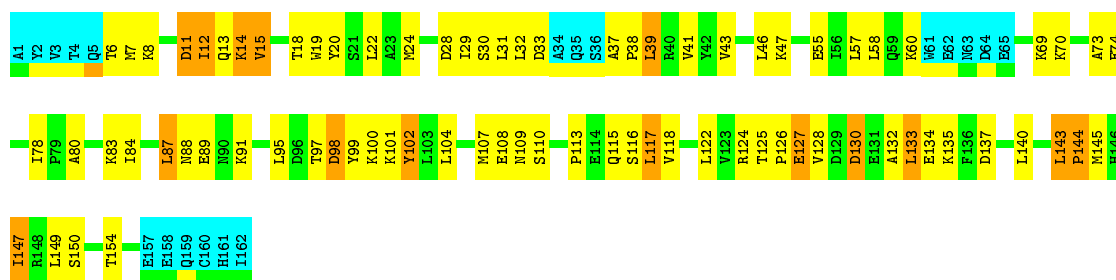
- Molecule 1: BETA-LACTOGLOBULIN



4.2.12 Score per residue for model 12

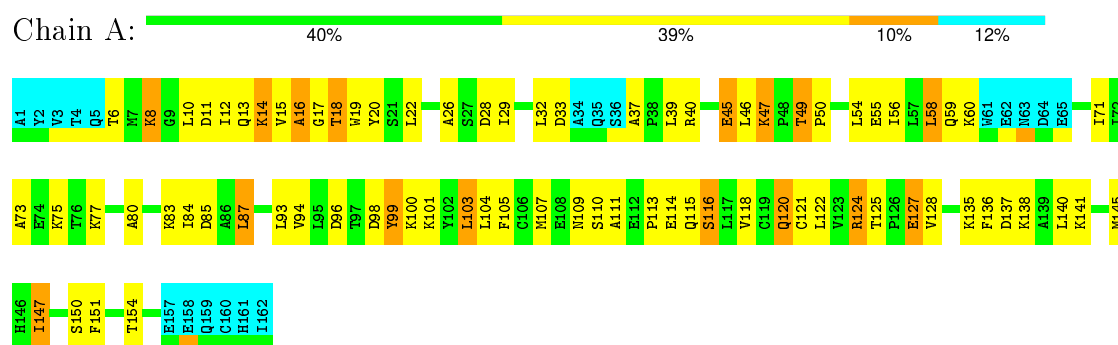
- Molecule 1: BETA-LACTOGLOBULIN





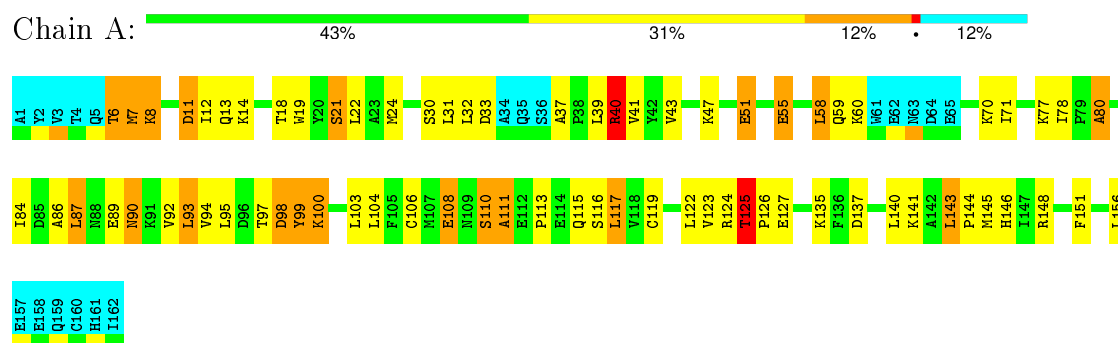
4.2.13 Score per residue for model 13

- Molecule 1: BETA-LACTOGLOBULIN



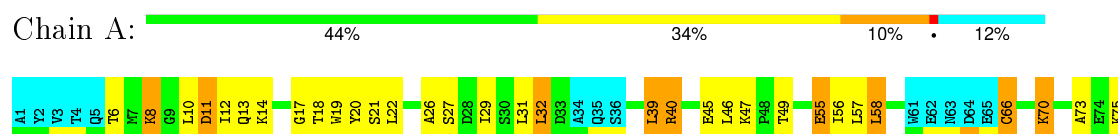
4.2.14 Score per residue for model 14

- Molecule 1: BETA-LACTOGLOBULIN



4.2.15 Score per residue for model 15

- Molecule 1: BETA-LACTOGLOBULIN

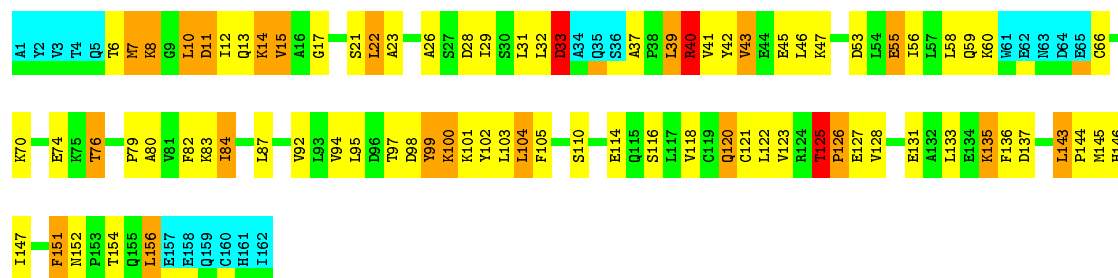




4.2.16 Score per residue for model 16

- Molecule 1: BETA-LACTOGLOBULIN

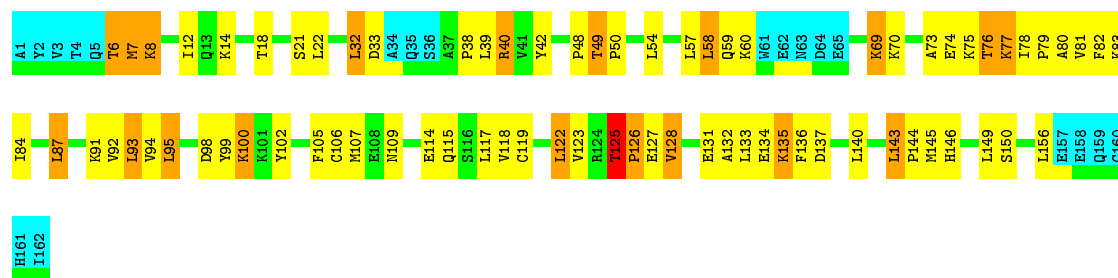
Chain A: 38% 36% 13% 12%



4.2.17 Score per residue for model 17

- Molecule 1: BETA-LACTOGLOBULIN

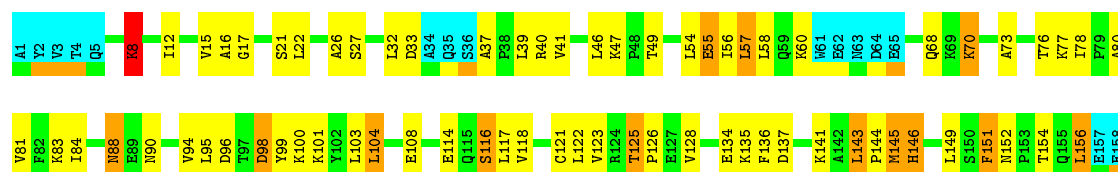
Chain A: 41% 35% 12% 12%



4.2.18 Score per residue for model 18

- Molecule 1: BETA-LACTOGLOBULIN

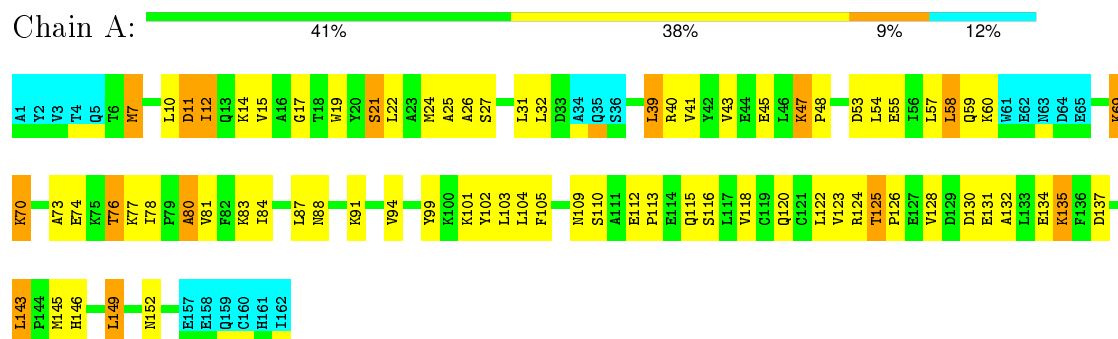
Chain A: 45% 35% 8% 12%





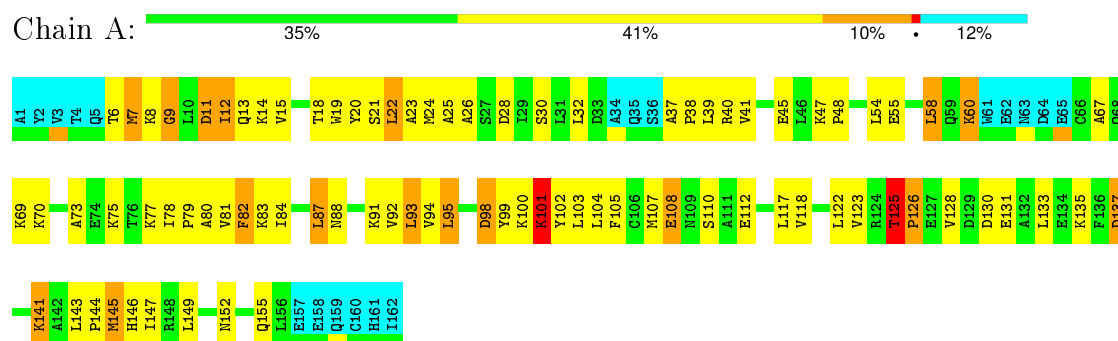
4.2.19 Score per residue for model 19

- Molecule 1: BETA-LACTOGLOBULIN



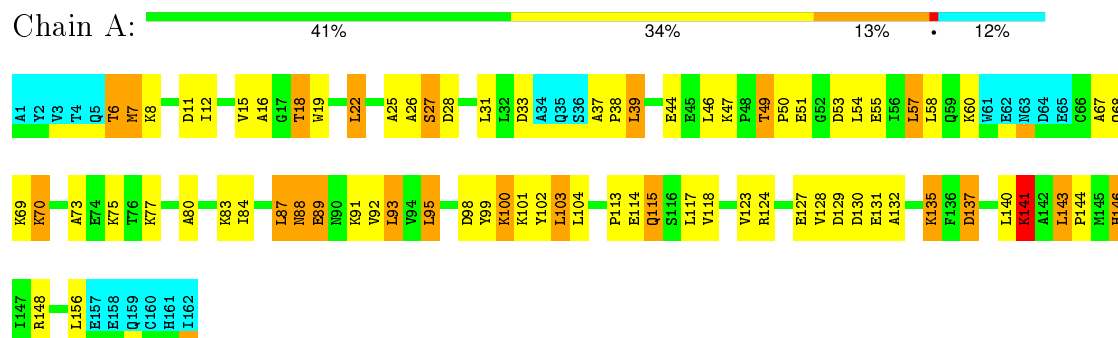
4.2.20 Score per residue for model 20

- Molecule 1: BETA-LACTOGLOBULIN



4.2.21 Score per residue for model 21

- Molecule 1: BETA-LACTOGLOBULIN



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 60 calculated structures, 21 were deposited, based on the following criterion: *lowest total energy*.

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

Software name	Classification	Version
X-PLOR	structure solution	ARIA
CNS	structure solution	0.9
CNS	refinement	0.9

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1127	1170	1169	41±9
All	All	23667	24570	24549	856

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 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:LEU:HD21	1:A:118:VAL:HG21	1.09	1.22	19	4
1:A:29:ILE:HG23	1:A:147:ILE:HD13	0.95	1.33	12	5
1:A:26:ALA:HB2	1:A:118:VAL:HG23	0.89	1.44	20	6
1:A:39:LEU:HD21	1:A:118:VAL:HG11	0.88	1.44	3	3
1:A:12:ILE:O	1:A:15:VAL:HG22	0.87	1.69	18	10
1:A:46:LEU:CD2	1:A:56:ILE:HG23	0.87	2.00	16	2
1:A:26:ALA:CB	1:A:118:VAL:HG12	0.87	2.00	9	3
1:A:123:VAL:HG21	1:A:127:GLU:O	0.84	1.72	14	1
1:A:41:VAL:CG2	1:A:58:LEU:HD13	0.84	2.03	11	1
1:A:39:LEU:HD11	1:A:118:VAL:HG11	0.81	1.51	7	3
1:A:26:ALA:HB1	1:A:118:VAL:HG12	0.81	1.52	9	1
1:A:23:ALA:HB3	1:A:121:CYS:SG	0.81	2.16	11	3
1:A:31:LEU:O	1:A:37:ALA:HB1	0.80	1.75	21	8
1:A:81:VAL:HG13	1:A:93:LEU:CD1	0.79	2.06	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ALA:HB1	1:A:145:MET:SD	0.79	2.18	6	6
1:A:12:ILE:HD11	1:A:54:LEU:HD13	0.79	1.53	21	4
1:A:93:LEU:HD21	1:A:108:GLU:OE2	0.78	1.78	20	1
1:A:39:LEU:CD2	1:A:118:VAL:HG21	0.78	2.08	15	3
1:A:28:ASP:HB2	1:A:31:LEU:HD22	0.78	1.53	1	1
1:A:103:LEU:HD11	1:A:122:LEU:HD12	0.78	1.54	2	1
1:A:32:LEU:HD22	1:A:149:LEU:CD1	0.77	2.10	17	1
1:A:123:VAL:HG11	1:A:126:PRO:O	0.77	1.80	2	1
1:A:43:VAL:HG11	1:A:122:LEU:HD11	0.76	1.58	6	1
1:A:46:LEU:HD21	1:A:56:ILE:HG23	0.74	1.59	16	1
1:A:103:LEU:O	1:A:103:LEU:HD13	0.74	1.80	2	1
1:A:92:VAL:C	1:A:93:LEU:HD12	0.74	2.02	5	1
1:A:46:LEU:HD11	1:A:54:LEU:HD11	0.74	1.59	4	1
1:A:93:LEU:HD11	1:A:108:GLU:OE2	0.74	1.83	14	2
1:A:10:LEU:HD11	1:A:79:PRO:CB	0.73	2.13	16	1
1:A:10:LEU:HD11	1:A:79:PRO:HB2	0.73	1.60	16	1
1:A:92:VAL:C	1:A:93:LEU:HD13	0.72	2.05	21	2
1:A:39:LEU:HD23	1:A:118:VAL:HG11	0.71	1.58	16	1
1:A:81:VAL:HG12	1:A:93:LEU:HG	0.71	1.62	15	1
1:A:10:LEU:O	1:A:10:LEU:HD23	0.71	1.84	13	2
1:A:39:LEU:HD22	1:A:118:VAL:HG21	0.71	1.60	16	3
1:A:73:ALA:HB1	1:A:82:PHE:HB3	0.71	1.59	17	2
1:A:56:ILE:HG22	1:A:58:LEU:CD2	0.71	2.16	15	1
1:A:41:VAL:HG21	1:A:58:LEU:HD13	0.70	1.60	11	1
1:A:101:LYS:O	1:A:123:VAL:HG23	0.70	1.85	8	2
1:A:81:VAL:HG22	1:A:93:LEU:CD1	0.70	2.17	4	1
1:A:139:ALA:O	1:A:143:LEU:HD21	0.70	1.87	4	1
1:A:31:LEU:HD22	1:A:39:LEU:HD23	0.69	1.62	7	1
1:A:22:LEU:HD11	1:A:128:VAL:HG23	0.69	1.64	5	2
1:A:20:TYR:O	1:A:122:LEU:HD23	0.69	1.87	13	2
1:A:54:LEU:HB3	1:A:73:ALA:HB3	0.68	1.65	11	14
1:A:31:LEU:HD13	1:A:118:VAL:CG2	0.68	2.19	6	1
1:A:46:LEU:CD1	1:A:56:ILE:HG23	0.68	2.18	15	3
1:A:58:LEU:HD12	1:A:69:LYS:O	0.68	1.88	19	4
1:A:31:LEU:HB3	1:A:39:LEU:HD13	0.67	1.64	3	1
1:A:22:LEU:CD1	1:A:128:VAL:HG22	0.67	2.18	19	1
1:A:39:LEU:CD2	1:A:118:VAL:HG11	0.67	2.18	16	3
1:A:10:LEU:HD12	1:A:94:VAL:HG11	0.67	1.67	19	1
1:A:121:CYS:O	1:A:122:LEU:HD23	0.67	1.90	2	1
1:A:57:LEU:HD22	1:A:70:LYS:HB3	0.67	1.65	21	1
1:A:19:TRP:CE3	1:A:103:LEU:HD12	0.67	2.25	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:LEU:HD22	1:A:118:VAL:HG11	0.66	1.67	6	2
1:A:81:VAL:HG22	1:A:93:LEU:HG	0.66	1.67	5	1
1:A:81:VAL:HG22	1:A:93:LEU:HD12	0.66	1.65	17	2
1:A:38:PRO:O	1:A:87:LEU:HD22	0.66	1.91	12	2
1:A:31:LEU:HD22	1:A:39:LEU:CD1	0.66	2.21	3	1
1:A:12:ILE:HG22	1:A:48:PRO:CG	0.66	2.20	4	5
1:A:12:ILE:HG22	1:A:48:PRO:HG3	0.66	1.66	4	4
1:A:11:ASP:O	1:A:15:VAL:HG23	0.66	1.91	19	1
1:A:92:VAL:O	1:A:93:LEU:HD13	0.66	1.91	17	1
1:A:12:ILE:HD11	1:A:79:PRO:O	0.65	1.91	11	1
1:A:26:ALA:HB2	1:A:118:VAL:HG13	0.65	1.68	16	1
1:A:95:LEU:HD11	1:A:104:LEU:HB3	0.65	1.67	20	2
1:A:143:LEU:N	1:A:143:LEU:HD22	0.65	2.07	10	1
1:A:121:CYS:SG	1:A:132:ALA:HB1	0.65	2.32	15	3
1:A:29:ILE:HG23	1:A:147:ILE:HD12	0.65	1.69	9	1
1:A:93:LEU:N	1:A:93:LEU:HD22	0.65	2.07	17	3
1:A:19:TRP:CD1	1:A:46:LEU:HD12	0.65	2.26	11	2
1:A:93:LEU:HD13	1:A:93:LEU:N	0.65	2.06	21	1
1:A:28:ASP:CB	1:A:31:LEU:HD22	0.64	2.22	1	1
1:A:39:LEU:O	1:A:41:VAL:HG22	0.64	1.93	14	4
1:A:22:LEU:HD22	1:A:22:LEU:O	0.64	1.93	20	1
1:A:46:LEU:HD23	1:A:56:ILE:HG23	0.64	1.70	16	1
1:A:125:THR:HG22	1:A:126:PRO:HD2	0.63	1.70	19	2
1:A:39:LEU:HD13	1:A:118:VAL:HG21	0.63	1.70	6	1
1:A:127:GLU:O	1:A:128:VAL:HG12	0.63	1.93	6	2
1:A:95:LEU:N	1:A:95:LEU:HD23	0.63	2.09	8	2
1:A:22:LEU:HD11	1:A:128:VAL:HG13	0.63	1.71	19	1
1:A:95:LEU:HD23	1:A:95:LEU:N	0.63	2.08	3	4
1:A:22:LEU:HD21	1:A:133:LEU:CD2	0.62	2.24	12	2
1:A:15:VAL:HG11	1:A:103:LEU:CD1	0.62	2.24	16	1
1:A:78:ILE:HD12	1:A:78:ILE:N	0.62	2.08	3	2
1:A:38:PRO:O	1:A:87:LEU:HD21	0.62	1.93	7	3
1:A:116:SER:O	1:A:118:VAL:HG22	0.62	1.95	18	1
1:A:32:LEU:HD11	1:A:39:LEU:HD23	0.62	1.70	9	1
1:A:54:LEU:HD23	1:A:56:ILE:CG1	0.62	2.25	2	1
1:A:39:LEU:CD1	1:A:118:VAL:HG11	0.61	2.23	7	2
1:A:31:LEU:HD12	1:A:118:VAL:CG2	0.61	2.25	16	1
1:A:18:THR:HG23	1:A:45:GLU:OE1	0.61	1.95	13	1
1:A:37:ALA:HB1	1:A:40:ARG:CB	0.61	2.25	11	2
1:A:73:ALA:HA	1:A:84:ILE:HG22	0.61	1.72	8	11
1:A:45:GLU:OE1	1:A:57:LEU:HD12	0.61	1.95	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:VAL:HG21	1:A:122:LEU:HD21	0.61	1.72	6	2
1:A:33:ASP:O	1:A:37:ALA:HB2	0.61	1.96	8	6
1:A:15:VAL:HG23	1:A:48:PRO:HD3	0.61	1.71	1	1
1:A:81:VAL:HG13	1:A:93:LEU:HD13	0.60	1.72	11	1
1:A:121:CYS:C	1:A:122:LEU:HD23	0.60	2.17	2	2
1:A:12:ILE:HD13	1:A:82:PHE:CZ	0.60	2.31	8	1
1:A:93:LEU:N	1:A:93:LEU:HD23	0.60	2.11	20	1
1:A:77:LYS:C	1:A:78:ILE:HD12	0.60	2.17	17	1
1:A:39:LEU:HD21	1:A:89:GLU:OE2	0.60	1.96	8	1
1:A:22:LEU:HD12	1:A:127:GLU:O	0.59	1.97	14	2
1:A:142:ALA:C	1:A:143:LEU:HD23	0.59	2.17	15	1
1:A:22:LEU:HD13	1:A:128:VAL:HG12	0.59	1.74	18	1
1:A:143:LEU:HD23	1:A:143:LEU:N	0.59	2.12	15	3
1:A:38:PRO:CB	1:A:87:LEU:HD13	0.59	2.27	17	1
1:A:128:VAL:HG13	1:A:128:VAL:O	0.59	1.97	16	1
1:A:20:TYR:C	1:A:122:LEU:HD23	0.59	2.17	13	1
1:A:46:LEU:CD1	1:A:54:LEU:HD11	0.59	2.27	4	1
1:A:31:LEU:HD12	1:A:39:LEU:HD23	0.59	1.74	19	1
1:A:29:ILE:HG22	1:A:33:ASP:HB3	0.59	1.75	6	1
1:A:22:LEU:HD21	1:A:128:VAL:HG13	0.58	1.75	17	1
1:A:84:ILE:HD11	1:A:89:GLU:O	0.58	1.97	11	4
1:A:26:ALA:O	1:A:147:ILE:HG22	0.58	1.98	15	2
1:A:37:ALA:HB1	1:A:40:ARG:HB2	0.58	1.76	20	4
1:A:56:ILE:HD12	1:A:71:ILE:O	0.58	1.98	13	1
1:A:80:ALA:O	1:A:94:VAL:HG23	0.58	1.98	18	5
1:A:118:VAL:HG13	1:A:118:VAL:O	0.57	1.99	21	1
1:A:143:LEU:N	1:A:143:LEU:HD23	0.57	2.14	8	5
1:A:84:ILE:HD11	1:A:89:GLU:OE1	0.57	1.99	21	1
1:A:10:LEU:CD1	1:A:94:VAL:HG11	0.57	2.29	19	1
1:A:26:ALA:HB2	1:A:118:VAL:CG2	0.57	2.30	5	2
1:A:152:ASN:O	1:A:156:LEU:HD23	0.57	2.00	7	1
1:A:81:VAL:HG13	1:A:81:VAL:O	0.57	2.00	9	1
1:A:39:LEU:HD13	1:A:39:LEU:O	0.56	2.01	2	2
1:A:32:LEU:HD22	1:A:149:LEU:HD13	0.56	1.77	10	1
1:A:39:LEU:HD21	1:A:118:VAL:CG2	0.56	2.31	18	2
1:A:84:ILE:H	1:A:84:ILE:HD13	0.56	1.59	11	2
1:A:41:VAL:HG21	1:A:58:LEU:HD22	0.56	1.77	5	1
1:A:121:CYS:C	1:A:122:LEU:HD12	0.56	2.21	18	1
1:A:22:LEU:CD2	1:A:132:ALA:HB3	0.56	2.31	19	1
1:A:22:LEU:C	1:A:22:LEU:HD13	0.56	2.22	20	1
1:A:7:MET:SD	1:A:97:THR:HG22	0.55	2.41	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:LEU:HD13	1:A:103:LEU:C	0.55	2.22	9	1
1:A:19:TRP:C	1:A:122:LEU:HD12	0.55	2.21	11	1
1:A:6:THR:O	1:A:80:ALA:HB1	0.55	2.01	11	1
1:A:31:LEU:HD22	1:A:39:LEU:CD2	0.55	2.31	7	1
1:A:31:LEU:HD13	1:A:118:VAL:HG11	0.55	1.76	9	1
1:A:103:LEU:C	1:A:103:LEU:HD22	0.55	2.20	2	1
1:A:103:LEU:HD22	1:A:103:LEU:C	0.55	2.21	13	1
1:A:78:ILE:HB	1:A:81:VAL:HG22	0.55	1.77	15	1
1:A:22:LEU:HD13	1:A:22:LEU:C	0.55	2.21	17	1
1:A:29:ILE:CG2	1:A:147:ILE:HD13	0.55	2.22	12	1
1:A:103:LEU:C	1:A:103:LEU:HD13	0.55	2.22	18	2
1:A:39:LEU:HG	1:A:118:VAL:HG11	0.55	1.78	11	1
1:A:15:VAL:HG13	1:A:19:TRP:CZ2	0.55	2.37	3	2
1:A:46:LEU:HD22	1:A:46:LEU:N	0.55	2.17	15	1
1:A:24:MET:SD	1:A:32:LEU:HD11	0.54	2.42	19	1
1:A:156:LEU:C	1:A:156:LEU:HD23	0.54	2.23	6	1
1:A:21:SER:HA	1:A:122:LEU:HD23	0.54	1.78	17	2
1:A:87:LEU:HD13	1:A:89:GLU:OE2	0.54	2.02	21	1
1:A:43:VAL:HG11	1:A:122:LEU:CD1	0.54	2.31	6	1
1:A:31:LEU:HD22	1:A:39:LEU:HD12	0.54	1.79	4	2
1:A:129:ASP:CG	1:A:132:ALA:HB3	0.54	2.23	21	1
1:A:38:PRO:CB	1:A:87:LEU:HD12	0.54	2.32	20	1
1:A:84:ILE:N	1:A:84:ILE:HD13	0.54	2.17	11	1
1:A:127:GLU:C	1:A:128:VAL:HG23	0.54	2.23	8	1
1:A:38:PRO:HB3	1:A:87:LEU:HD13	0.54	1.79	17	1
1:A:156:LEU:C	1:A:156:LEU:HD12	0.53	2.24	14	1
1:A:19:TRP:CZ3	1:A:103:LEU:HD12	0.53	2.37	2	2
1:A:151:PHE:CB	1:A:156:LEU:HD12	0.53	2.33	6	1
1:A:22:LEU:HD12	1:A:123:VAL:HG21	0.53	1.78	21	1
1:A:46:LEU:HD11	1:A:56:ILE:HG23	0.53	1.78	15	2
1:A:22:LEU:C	1:A:22:LEU:HD23	0.53	2.24	5	2
1:A:22:LEU:HD23	1:A:22:LEU:C	0.53	2.24	14	1
1:A:147:ILE:HG23	1:A:147:ILE:O	0.53	2.04	7	2
1:A:105:PHE:CE1	1:A:122:LEU:HD12	0.53	2.39	13	1
1:A:121:CYS:O	1:A:122:LEU:HD12	0.52	2.04	8	1
1:A:97:THR:HG21	1:A:103:LEU:HD12	0.52	1.80	14	1
1:A:76:THR:O	1:A:76:THR:HG22	0.52	2.04	18	1
1:A:12:ILE:HG22	1:A:48:PRO:HG2	0.52	1.81	1	1
1:A:14:LYS:CD	1:A:99:TYR:CE1	0.52	2.92	16	1
1:A:12:ILE:HD12	1:A:82:PHE:CZ	0.52	2.39	11	1
1:A:156:LEU:O	1:A:156:LEU:HD23	0.52	2.05	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:LEU:HD21	1:A:80:ALA:HA	0.52	1.81	11	1
1:A:105:PHE:CE2	1:A:120:GLN:CG	0.52	2.93	10	1
1:A:105:PHE:CE1	1:A:122:LEU:HD11	0.52	2.40	17	1
1:A:57:LEU:HD23	1:A:69:LYS:O	0.52	2.04	2	1
1:A:149:LEU:HD12	1:A:151:PHE:CE1	0.52	2.40	11	1
1:A:97:THR:O	1:A:102:TYR:CE1	0.52	2.63	8	1
1:A:29:ILE:HA	1:A:147:ILE:HG21	0.51	1.81	15	1
1:A:19:TRP:CE3	1:A:103:LEU:HD23	0.51	2.39	4	1
1:A:18:THR:HG23	1:A:18:THR:O	0.51	2.05	5	1
1:A:37:ALA:HB3	1:A:40:ARG:HB2	0.51	1.82	7	1
1:A:22:LEU:HD11	1:A:128:VAL:HG22	0.51	1.82	10	1
1:A:44:GLU:OE2	1:A:57:LEU:HD22	0.51	2.05	2	1
1:A:84:ILE:HD12	1:A:92:VAL:CG2	0.51	2.36	16	1
1:A:84:ILE:HD13	1:A:84:ILE:N	0.51	2.20	16	1
1:A:82:PHE:N	1:A:82:PHE:CD1	0.51	2.78	20	2
1:A:14:LYS:NZ	1:A:99:TYR:CE2	0.51	2.79	17	1
1:A:105:PHE:CZ	1:A:120:GLN:CG	0.51	2.94	10	2
1:A:22:LEU:HD21	1:A:133:LEU:HD22	0.51	1.83	12	1
1:A:29:ILE:HG22	1:A:33:ASP:HB2	0.51	1.83	2	2
1:A:26:ALA:HA	1:A:118:VAL:HG12	0.50	1.82	18	2
1:A:41:VAL:HG12	1:A:60:LYS:CB	0.50	2.36	9	1
1:A:93:LEU:HD13	1:A:108:GLU:OE2	0.50	2.05	5	1
1:A:81:VAL:HG22	1:A:93:LEU:HD11	0.50	1.83	4	1
1:A:128:VAL:HG22	1:A:128:VAL:O	0.50	2.05	9	1
1:A:147:ILE:O	1:A:147:ILE:HG23	0.50	2.06	10	1
1:A:103:LEU:HD11	1:A:122:LEU:CB	0.50	2.36	13	1
1:A:118:VAL:O	1:A:118:VAL:HG13	0.50	2.07	15	3
1:A:39:LEU:HD21	1:A:118:VAL:CG1	0.50	2.29	3	1
1:A:104:LEU:HD22	1:A:121:CYS:SG	0.50	2.46	2	1
1:A:107:MET:O	1:A:118:VAL:HG12	0.50	2.06	13	1
1:A:49:THR:HG1	1:A:53:ASP:CG	0.50	2.09	8	1
1:A:151:PHE:N	1:A:151:PHE:CD1	0.50	2.80	16	1
1:A:31:LEU:C	1:A:37:ALA:HB1	0.50	2.26	1	2
1:A:151:PHE:HB3	1:A:156:LEU:HD12	0.50	1.84	6	2
1:A:28:ASP:HB3	1:A:31:LEU:HD22	0.50	1.84	8	1
1:A:43:VAL:HG11	1:A:122:LEU:HD21	0.50	1.83	12	2
1:A:15:VAL:HG11	1:A:103:LEU:HD13	0.50	1.83	8	2
1:A:28:ASP:OD2	1:A:31:LEU:HD13	0.50	2.07	8	1
1:A:56:ILE:O	1:A:58:LEU:HD23	0.49	2.07	13	1
1:A:8:LYS:H	1:A:80:ALA:HB2	0.49	1.66	1	3
1:A:7:MET:SD	1:A:10:LEU:HD12	0.49	2.47	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:PRO:HG3	1:A:54:LEU:HD12	0.49	1.85	2	1
1:A:32:LEU:O	1:A:32:LEU:HD12	0.49	2.07	6	1
1:A:39:LEU:CD1	1:A:118:VAL:HG21	0.49	2.38	2	3
1:A:151:PHE:CD1	1:A:151:PHE:N	0.49	2.78	18	2
1:A:31:LEU:HD13	1:A:39:LEU:HD13	0.49	1.85	6	1
1:A:143:LEU:CB	1:A:144:PRO:CD	0.49	2.90	2	6
1:A:123:VAL:HG21	1:A:127:GLU:HA	0.49	1.83	17	1
1:A:128:VAL:HG23	1:A:128:VAL:O	0.49	2.08	20	1
1:A:78:ILE:HB	1:A:81:VAL:HG12	0.49	1.85	18	3
1:A:31:LEU:HD22	1:A:39:LEU:HD13	0.49	1.84	3	1
1:A:10:LEU:HD23	1:A:79:PRO:O	0.49	2.07	15	1
1:A:12:ILE:HD12	1:A:82:PHE:HZ	0.48	1.67	11	1
1:A:21:SER:O	1:A:156:LEU:HD21	0.48	2.08	16	1
1:A:103:LEU:CD1	1:A:103:LEU:N	0.48	2.76	13	1
1:A:7:MET:HB3	1:A:80:ALA:HB2	0.48	1.85	21	1
1:A:14:LYS:CD	1:A:99:TYR:CD1	0.48	2.96	12	1
1:A:125:THR:N	1:A:126:PRO:CD	0.48	2.76	8	1
1:A:86:ALA:C	1:A:87:LEU:HD23	0.48	2.29	14	1
1:A:43:VAL:HG22	1:A:58:LEU:CD1	0.48	2.38	16	1
1:A:84:ILE:CD1	1:A:84:ILE:N	0.48	2.77	16	1
1:A:32:LEU:HD21	1:A:149:LEU:HG	0.48	1.84	19	1
1:A:81:VAL:HG23	1:A:93:LEU:HD21	0.48	1.84	9	1
1:A:104:LEU:HD11	1:A:121:CYS:SG	0.48	2.49	7	2
1:A:22:LEU:HD11	1:A:133:LEU:HD12	0.48	1.86	20	1
1:A:41:VAL:HG23	1:A:41:VAL:O	0.48	2.08	10	1
1:A:103:LEU:HD22	1:A:103:LEU:O	0.48	2.09	13	1
1:A:54:LEU:HD23	1:A:56:ILE:HG12	0.48	1.84	2	1
1:A:116:SER:O	1:A:118:VAL:HG12	0.48	2.08	7	1
1:A:125:THR:CB	1:A:126:PRO:CD	0.48	2.92	2	8
1:A:92:VAL:C	1:A:93:LEU:HD22	0.48	2.30	4	1
1:A:17:GLY:O	1:A:19:TRP:CD1	0.47	2.68	11	2
1:A:41:VAL:CG1	1:A:58:LEU:HD13	0.47	2.39	1	1
1:A:31:LEU:CD1	1:A:118:VAL:CG2	0.47	2.92	6	2
1:A:32:LEU:HD23	1:A:40:ARG:HB2	0.47	1.85	9	1
1:A:19:TRP:CH2	1:A:103:LEU:HD12	0.47	2.44	13	1
1:A:81:VAL:HG22	1:A:93:LEU:CG	0.47	2.39	5	1
1:A:23:ALA:HB1	1:A:149:LEU:O	0.47	2.09	3	1
1:A:27:SER:O	1:A:146:HIS:CG	0.47	2.67	21	1
1:A:14:LYS:HD2	1:A:99:TYR:CE1	0.47	2.45	16	1
1:A:105:PHE:CD1	1:A:105:PHE:N	0.47	2.81	13	1
1:A:79:PRO:O	1:A:82:PHE:CZ	0.47	2.68	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:ILE:CD1	1:A:78:ILE:N	0.47	2.77	17	2
1:A:71:ILE:HD11	1:A:87:LEU:HD13	0.47	1.85	5	1
1:A:143:LEU:HD12	1:A:145:MET:CE	0.47	2.40	4	1
1:A:38:PRO:CA	1:A:87:LEU:CD1	0.47	2.92	20	1
1:A:19:TRP:CH2	1:A:99:TYR:O	0.47	2.68	11	5
1:A:143:LEU:HD23	1:A:144:PRO:HD2	0.47	1.87	18	2
1:A:41:VAL:HG11	1:A:58:LEU:HD21	0.47	1.86	16	1
1:A:10:LEU:HD22	1:A:12:ILE:HD13	0.47	1.86	19	1
1:A:12:ILE:HG22	1:A:48:PRO:CB	0.47	2.39	19	1
1:A:57:LEU:HD12	1:A:70:LYS:HB3	0.47	1.86	19	1
1:A:26:ALA:HB2	1:A:118:VAL:HG12	0.47	1.84	9	1
1:A:31:LEU:HD13	1:A:118:VAL:HG21	0.47	1.87	6	1
1:A:19:TRP:CZ2	1:A:99:TYR:O	0.47	2.68	20	2
1:A:32:LEU:CD1	1:A:40:ARG:N	0.47	2.78	7	1
1:A:16:ALA:HB1	1:A:47:LYS:HG3	0.47	1.86	21	3
1:A:81:VAL:HG23	1:A:93:LEU:CD2	0.47	2.40	2	2
1:A:22:LEU:HD13	1:A:127:GLU:O	0.47	2.09	9	1
1:A:84:ILE:CD1	1:A:88:ASN:ND2	0.47	2.78	20	1
1:A:24:MET:CB	1:A:32:LEU:HD21	0.47	2.40	14	1
1:A:28:ASP:HB3	1:A:31:LEU:HD13	0.47	1.86	1	1
1:A:39:LEU:CD2	1:A:118:VAL:CG1	0.47	2.93	16	1
1:A:18:THR:O	1:A:19:TRP:CG	0.47	2.68	21	1
1:A:46:LEU:HD12	1:A:56:ILE:HG13	0.46	1.86	9	1
1:A:103:LEU:HD13	1:A:103:LEU:N	0.46	2.25	13	1
1:A:14:LYS:CB	1:A:99:TYR:CD1	0.46	2.98	13	1
1:A:79:PRO:O	1:A:82:PHE:CE1	0.46	2.68	8	1
1:A:31:LEU:O	1:A:32:LEU:HD12	0.46	2.10	7	1
1:A:94:VAL:HG13	1:A:104:LEU:O	0.46	2.11	10	2
1:A:152:ASN:CB	1:A:153:PRO:CD	0.46	2.93	5	2
1:A:76:THR:CG2	1:A:81:VAL:HG13	0.46	2.40	18	1
1:A:25:ALA:HB2	1:A:148:ARG:HG3	0.46	1.87	21	1
1:A:31:LEU:CB	1:A:39:LEU:HD13	0.46	2.38	3	1
1:A:10:LEU:HD23	1:A:12:ILE:N	0.46	2.26	19	1
1:A:39:LEU:HD21	1:A:89:GLU:OE1	0.46	2.11	11	1
1:A:22:LEU:CD2	1:A:132:ALA:CB	0.46	2.93	19	1
1:A:79:PRO:O	1:A:82:PHE:CE2	0.46	2.68	15	3
1:A:112:GLU:N	1:A:113:PRO:CD	0.46	2.79	19	1
1:A:125:THR:N	1:A:126:PRO:HD3	0.46	2.25	8	1
1:A:122:LEU:HD12	1:A:122:LEU:N	0.46	2.26	14	1
1:A:21:SER:HB3	1:A:43:VAL:HG12	0.46	1.87	14	2
1:A:18:THR:O	1:A:18:THR:HG23	0.46	2.11	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:PHE:CE1	1:A:120:GLN:CG	0.46	2.98	16	1
1:A:6:THR:O	1:A:6:THR:HG23	0.45	2.12	11	1
1:A:76:THR:HG21	1:A:81:VAL:HG13	0.45	1.88	18	2
1:A:11:ASP:O	1:A:13:GLN:N	0.45	2.49	16	11
1:A:58:LEU:HD21	1:A:71:ILE:CD1	0.45	2.41	3	1
1:A:104:LEU:N	1:A:104:LEU:HD23	0.45	2.26	11	1
1:A:49:THR:HG22	1:A:50:PRO:HD2	0.45	1.87	13	3
1:A:93:LEU:N	1:A:93:LEU:CD2	0.45	2.78	13	2
1:A:143:LEU:CB	1:A:144:PRO:HD2	0.45	2.41	16	14
1:A:32:LEU:HD11	1:A:40:ARG:N	0.45	2.26	7	1
1:A:10:LEU:HD23	1:A:10:LEU:C	0.45	2.32	19	1
1:A:105:PHE:CZ	1:A:120:GLN:NE2	0.45	2.83	19	1
1:A:105:PHE:CZ	1:A:120:GLN:HG2	0.45	2.45	13	1
1:A:57:LEU:HD22	1:A:70:LYS:CB	0.45	2.42	18	1
1:A:19:TRP:CZ3	1:A:103:LEU:HD23	0.45	2.46	21	1
1:A:58:LEU:HD11	1:A:71:ILE:CD1	0.45	2.41	14	1
1:A:42:TYR:CE2	1:A:44:GLU:OE2	0.45	2.70	9	1
1:A:20:TYR:O	1:A:122:LEU:HD13	0.45	2.11	11	1
1:A:26:ALA:CA	1:A:118:VAL:HG12	0.45	2.42	18	1
1:A:48:PRO:HG3	1:A:54:LEU:HD13	0.45	1.89	8	1
1:A:95:LEU:CD2	1:A:95:LEU:N	0.45	2.78	8	2
1:A:32:LEU:HD13	1:A:40:ARG:HG2	0.45	1.88	16	1
1:A:22:LEU:O	1:A:22:LEU:HD23	0.45	2.12	21	1
1:A:78:ILE:HG23	1:A:78:ILE:O	0.45	2.10	5	1
1:A:76:THR:HG23	1:A:81:VAL:HG13	0.45	1.88	8	1
1:A:143:LEU:HB3	1:A:144:PRO:CD	0.45	2.42	2	2
1:A:140:LEU:O	1:A:143:LEU:HD12	0.45	2.12	21	2
1:A:43:VAL:CG1	1:A:122:LEU:HD11	0.45	2.38	6	1
1:A:143:LEU:N	1:A:143:LEU:CD2	0.45	2.78	10	1
1:A:105:PHE:CZ	1:A:120:GLN:HG3	0.45	2.47	10	1
1:A:31:LEU:HD13	1:A:39:LEU:CD1	0.45	2.42	4	1
1:A:32:LEU:HB2	1:A:147:ILE:HD13	0.44	1.87	20	1
1:A:14:LYS:HD2	1:A:99:TYR:CG	0.44	2.47	12	2
1:A:105:PHE:CE1	1:A:120:GLN:HG3	0.44	2.47	16	1
1:A:11:ASP:OD2	1:A:99:TYR:CZ	0.44	2.70	19	1
1:A:39:LEU:HD22	1:A:118:VAL:CG1	0.44	2.40	6	1
1:A:39:LEU:HD11	1:A:118:VAL:CG1	0.44	2.42	5	1
1:A:19:TRP:CZ3	1:A:103:LEU:HB2	0.44	2.48	5	1
1:A:125:THR:CB	1:A:126:PRO:HD3	0.44	2.42	20	6
1:A:38:PRO:CB	1:A:87:LEU:CD1	0.44	2.95	20	1
1:A:20:TYR:N	1:A:20:TYR:CD1	0.44	2.86	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:LEU:HD23	1:A:56:ILE:HA	0.44	1.88	3	2
1:A:41:VAL:CG1	1:A:58:LEU:HD21	0.44	2.42	16	1
1:A:121:CYS:SG	1:A:136:PHE:CD1	0.44	3.10	1	2
1:A:79:PRO:O	1:A:80:ALA:HB2	0.44	2.13	5	1
1:A:105:PHE:N	1:A:105:PHE:CD1	0.44	2.85	20	1
1:A:152:ASN:O	1:A:156:LEU:N	0.44	2.51	9	1
1:A:121:CYS:HB2	1:A:136:PHE:CD1	0.44	2.48	7	4
1:A:56:ILE:HG22	1:A:58:LEU:HD22	0.44	1.89	15	1
1:A:127:GLU:O	1:A:128:VAL:CG1	0.44	2.65	6	2
1:A:29:ILE:O	1:A:33:ASP:N	0.43	2.51	16	3
1:A:125:THR:HG23	1:A:127:GLU:O	0.43	2.13	5	1
1:A:95:LEU:HD11	1:A:104:LEU:CB	0.43	2.40	20	2
1:A:109:ASN:O	1:A:111:ALA:N	0.43	2.52	7	7
1:A:98:ASP:OD1	1:A:102:TYR:CZ	0.43	2.71	15	1
1:A:149:LEU:N	1:A:149:LEU:HD22	0.43	2.29	6	1
1:A:93:LEU:HD23	1:A:93:LEU:N	0.43	2.29	1	1
1:A:121:CYS:SG	1:A:136:PHE:CG	0.43	3.11	16	1
1:A:25:ALA:HB3	1:A:140:LEU:HD21	0.43	1.89	21	2
1:A:32:LEU:N	1:A:32:LEU:HD12	0.43	2.28	4	1
1:A:93:LEU:CD2	1:A:93:LEU:N	0.43	2.82	9	2
1:A:102:TYR:CD2	1:A:132:ALA:CB	0.43	3.01	8	1
1:A:31:LEU:HB2	1:A:32:LEU:HD12	0.43	1.90	4	1
1:A:110:SER:O	1:A:111:ALA:HB2	0.43	2.14	8	3
1:A:22:LEU:HD13	1:A:132:ALA:HB3	0.43	1.91	1	2
1:A:23:ALA:CB	1:A:136:PHE:CE2	0.43	3.02	5	1
1:A:19:TRP:C	1:A:20:TYR:CD1	0.43	2.92	2	5
1:A:6:THR:O	1:A:8:LYS:N	0.43	2.52	11	6
1:A:152:ASN:O	1:A:156:LEU:CB	0.43	2.67	6	1
1:A:154:THR:O	1:A:155:GLN:CB	0.43	2.66	6	1
1:A:47:LYS:O	1:A:55:GLU:CB	0.43	2.67	14	13
1:A:78:ILE:O	1:A:80:ALA:N	0.43	2.49	14	5
1:A:150:SER:C	1:A:151:PHE:CD1	0.43	2.92	13	1
1:A:104:LEU:HD22	1:A:136:PHE:CD1	0.43	2.49	4	1
1:A:22:LEU:HD21	1:A:133:LEU:CD1	0.43	2.43	20	1
1:A:7:MET:N	1:A:94:VAL:O	0.43	2.52	11	4
1:A:132:ALA:O	1:A:136:PHE:CB	0.43	2.67	17	2
1:A:22:LEU:HD21	1:A:133:LEU:HD12	0.43	1.90	1	1
1:A:76:THR:O	1:A:77:LYS:CB	0.43	2.67	18	1
1:A:48:PRO:CB	1:A:53:ASP:O	0.43	2.67	6	1
1:A:98:ASP:O	1:A:100:LYS:N	0.42	2.53	7	16
1:A:54:LEU:HD23	1:A:56:ILE:HD11	0.42	1.91	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LEU:O	1:A:37:ALA:CB	0.42	2.67	16	1
1:A:19:TRP:CZ3	1:A:124:ARG:N	0.42	2.87	13	1
1:A:143:LEU:O	1:A:145:MET:N	0.42	2.52	20	1
1:A:137:ASP:O	1:A:141:LYS:N	0.42	2.52	20	3
1:A:102:TYR:CD2	1:A:132:ALA:HB2	0.42	2.50	12	2
1:A:104:LEU:HD22	1:A:121:CYS:HB3	0.42	1.90	16	1
1:A:105:PHE:CZ	1:A:120:GLN:CD	0.42	2.93	19	1
1:A:129:ASP:O	1:A:131:GLU:N	0.42	2.52	6	4
1:A:103:LEU:CD1	1:A:122:LEU:CB	0.42	2.97	13	1
1:A:113:PRO:O	1:A:115:GLN:N	0.42	2.52	21	2
1:A:101:LYS:CG	1:A:131:GLU:OE1	0.42	2.68	20	1
1:A:24:MET:O	1:A:149:LEU:N	0.42	2.53	8	2
1:A:113:PRO:O	1:A:117:LEU:N	0.42	2.52	11	5
1:A:39:LEU:CD1	1:A:39:LEU:O	0.42	2.68	19	1
1:A:103:LEU:HD11	1:A:122:LEU:HB3	0.42	1.90	13	1
1:A:6:THR:O	1:A:80:ALA:CB	0.42	2.68	16	5
1:A:22:LEU:CD1	1:A:127:GLU:O	0.42	2.68	7	3
1:A:19:TRP:CD1	1:A:19:TRP:N	0.42	2.87	14	1
1:A:31:LEU:O	1:A:39:LEU:CB	0.42	2.68	10	3
1:A:140:LEU:O	1:A:143:LEU:CD1	0.42	2.67	2	2
1:A:7:MET:CE	1:A:99:TYR:OH	0.42	2.68	16	1
1:A:128:VAL:O	1:A:128:VAL:HG13	0.42	2.15	9	1
1:A:145:MET:O	1:A:146:HIS:CG	0.42	2.73	18	1
1:A:98:ASP:CG	1:A:102:TYR:CE2	0.42	2.92	5	1
1:A:44:GLU:OE2	1:A:59:GLN:CG	0.42	2.68	11	1
1:A:42:TYR:CB	1:A:59:GLN:O	0.42	2.68	17	1
1:A:12:ILE:CG2	1:A:48:PRO:CG	0.42	2.95	1	1
1:A:19:TRP:O	1:A:20:TYR:CG	0.42	2.73	15	1
1:A:42:TYR:CE1	1:A:156:LEU:HD11	0.42	2.50	9	1
1:A:21:SER:O	1:A:156:LEU:CD1	0.42	2.68	18	1
1:A:39:LEU:HD21	1:A:89:GLU:CD	0.42	2.35	8	1
1:A:81:VAL:O	1:A:82:PHE:CG	0.42	2.72	4	1
1:A:92:VAL:C	1:A:93:LEU:HD23	0.42	2.35	20	1
1:A:27:SER:O	1:A:146:HIS:ND1	0.42	2.53	10	1
1:A:125:THR:O	1:A:127:GLU:N	0.42	2.53	12	2
1:A:143:LEU:HB3	1:A:144:PRO:HD2	0.42	1.91	2	2
1:A:84:ILE:CD1	1:A:89:GLU:O	0.42	2.68	1	1
1:A:27:SER:O	1:A:146:HIS:CB	0.42	2.68	9	3
1:A:80:ALA:O	1:A:94:VAL:N	0.42	2.53	18	1
1:A:18:THR:CG2	1:A:18:THR:O	0.42	2.68	5	1
1:A:100:LYS:O	1:A:101:LYS:CD	0.42	2.68	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:GLU:O	1:A:135:LYS:CE	0.42	2.68	1	2
1:A:17:GLY:O	1:A:45:GLU:CG	0.42	2.68	16	2
1:A:102:TYR:CZ	1:A:135:LYS:HD2	0.42	2.50	16	2
1:A:95:LEU:CD1	1:A:104:LEU:CB	0.42	2.98	15	1
1:A:102:TYR:CB	1:A:122:LEU:O	0.42	2.68	19	2
1:A:22:LEU:O	1:A:151:PHE:N	0.42	2.53	13	1
1:A:123:VAL:CG1	1:A:129:ASP:OD2	0.42	2.68	21	1
1:A:24:MET:CE	1:A:41:VAL:O	0.42	2.68	19	2
1:A:53:ASP:CB	1:A:73:ALA:O	0.42	2.68	2	2
1:A:31:LEU:CD1	1:A:118:VAL:HG21	0.42	2.45	16	1
1:A:14:LYS:HD3	1:A:99:TYR:CE1	0.42	2.50	16	1
1:A:98:ASP:O	1:A:100:LYS:CG	0.42	2.67	9	2
1:A:101:LYS:O	1:A:124:ARG:N	0.42	2.53	9	1
1:A:39:LEU:O	1:A:41:VAL:N	0.42	2.53	18	1
1:A:32:LEU:HD13	1:A:40:ARG:HA	0.42	1.90	14	1
1:A:22:LEU:HD12	1:A:123:VAL:HG11	0.42	1.91	3	1
1:A:75:LYS:O	1:A:76:THR:CG2	0.42	2.68	4	1
1:A:12:ILE:O	1:A:15:VAL:CG2	0.42	2.68	20	2
1:A:95:LEU:HD11	1:A:119:CYS:SG	0.42	2.55	10	1
1:A:18:THR:O	1:A:124:ARG:CG	0.42	2.68	12	1
1:A:109:ASN:O	1:A:113:PRO:CD	0.42	2.68	12	1
1:A:14:LYS:HB3	1:A:99:TYR:CD1	0.42	2.50	7	1
1:A:102:TYR:OH	1:A:135:LYS:CD	0.41	2.68	21	4
1:A:103:LEU:HD23	1:A:103:LEU:C	0.41	2.36	16	1
1:A:97:THR:HG23	1:A:99:TYR:CE1	0.41	2.50	16	1
1:A:12:ILE:CG2	1:A:48:PRO:HB3	0.41	2.45	19	1
1:A:22:LEU:HD13	1:A:23:ALA:CB	0.41	2.45	20	1
1:A:41:VAL:HG23	1:A:58:LEU:HD13	0.41	1.86	11	1
1:A:15:VAL:O	1:A:17:GLY:N	0.41	2.53	13	2
1:A:32:LEU:O	1:A:32:LEU:CD1	0.41	2.68	6	1
1:A:46:LEU:HD12	1:A:55:GLU:O	0.41	2.15	4	1
1:A:103:LEU:C	1:A:104:LEU:HD23	0.41	2.36	14	1
1:A:140:LEU:HD13	1:A:143:LEU:HD12	0.41	1.91	14	1
1:A:41:VAL:HG11	1:A:58:LEU:HD13	0.41	1.92	1	1
1:A:32:LEU:HD12	1:A:39:LEU:HD22	0.41	1.92	15	1
1:A:95:LEU:HD11	1:A:104:LEU:HD23	0.41	1.91	7	1
1:A:110:SER:OG	1:A:111:ALA:N	0.41	2.53	7	1
1:A:31:LEU:O	1:A:37:ALA:CB	0.41	2.67	5	1
1:A:39:LEU:CD2	1:A:118:VAL:CG2	0.41	2.97	16	1
1:A:53:ASP:OD1	1:A:53:ASP:N	0.41	2.53	19	1
1:A:60:LYS:O	1:A:67:ALA:N	0.41	2.53	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:THR:OG1	1:A:98:ASP:N	0.41	2.54	12	1
1:A:23:ALA:HB1	1:A:136:PHE:CE2	0.41	2.50	5	1
1:A:124:ARG:O	1:A:125:THR:CB	0.41	2.69	8	1
1:A:103:LEU:CD1	1:A:122:LEU:HB2	0.41	2.46	13	1
1:A:46:LEU:HD12	1:A:56:ILE:HA	0.41	1.93	13	1
1:A:129:ASP:OD1	1:A:132:ALA:HB3	0.41	2.15	21	1
1:A:14:LYS:HE3	1:A:99:TYR:CD2	0.41	2.50	5	1
1:A:84:ILE:HD13	1:A:92:VAL:HG21	0.41	1.93	14	1
1:A:152:ASN:OD1	1:A:153:PRO:CD	0.41	2.69	11	1
1:A:78:ILE:HG22	1:A:80:ALA:H	0.41	1.75	12	1
1:A:107:MET:N	1:A:118:VAL:O	0.41	2.54	13	1
1:A:95:LEU:CD2	1:A:104:LEU:O	0.41	2.69	21	1
1:A:98:ASP:O	1:A:99:TYR:CB	0.41	2.69	4	1
1:A:101:LYS:CG	1:A:131:GLU:OE2	0.41	2.68	1	1
1:A:121:CYS:HB3	1:A:136:PHE:CD1	0.41	2.51	16	1
1:A:32:LEU:O	1:A:37:ALA:HB2	0.41	2.15	16	1
1:A:56:ILE:O	1:A:70:LYS:CB	0.41	2.69	15	1
1:A:10:LEU:CD2	1:A:79:PRO:O	0.41	2.69	15	1
1:A:127:GLU:O	1:A:128:VAL:O	0.41	2.39	6	1
1:A:119:CYS:O	1:A:120:GLN:CG	0.41	2.68	6	1
1:A:12:ILE:CG2	1:A:48:PRO:CB	0.41	2.99	5	1
1:A:39:LEU:HD12	1:A:118:VAL:HG21	0.41	1.92	5	1
1:A:58:LEU:CD1	1:A:69:LYS:O	0.41	2.67	4	1
1:A:43:VAL:HG22	1:A:58:LEU:HD11	0.41	1.94	16	1
1:A:87:LEU:O	1:A:89:GLU:N	0.41	2.54	5	1
1:A:44:GLU:N	1:A:57:LEU:O	0.41	2.54	8	1
1:A:39:LEU:HD21	1:A:118:VAL:CB	0.40	2.47	17	1
1:A:75:LYS:CG	1:A:75:LYS:O	0.40	2.69	15	1
1:A:32:LEU:HD23	1:A:40:ARG:CB	0.40	2.46	9	1
1:A:8:LYS:N	1:A:80:ALA:HB2	0.40	2.30	18	1
1:A:103:LEU:O	1:A:104:LEU:HD23	0.40	2.16	14	1
1:A:43:VAL:HG21	1:A:122:LEU:CD2	0.40	2.46	14	1
1:A:128:VAL:O	1:A:128:VAL:CG1	0.40	2.68	16	1
1:A:76:THR:OG1	1:A:77:LYS:N	0.40	2.54	19	2
1:A:31:LEU:CD2	1:A:88:ASN:CB	0.40	2.99	21	1
1:A:100:LYS:CG	1:A:100:LYS:O	0.40	2.69	5	1
1:A:7:MET:CE	1:A:9:GLY:O	0.40	2.69	20	1
1:A:103:LEU:O	1:A:122:LEU:N	0.40	2.53	11	1
1:A:123:VAL:HG11	1:A:128:VAL:H	0.40	1.75	17	1
1:A:98:ASP:OD2	1:A:101:LYS:CD	0.40	2.69	2	1
1:A:48:PRO:CA	1:A:53:ASP:O	0.40	2.69	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:VAL:HG12	1:A:124:ARG:N	0.40	2.31	14	1
1:A:112:GLU:CG	1:A:112:GLU:O	0.40	2.69	10	1
1:A:15:VAL:HG12	1:A:15:VAL:O	0.40	2.17	3	1
1:A:39:LEU:CD2	1:A:118:VAL:CB	0.40	2.98	16	1
1:A:56:ILE:HG22	1:A:58:LEU:HD23	0.40	1.91	15	1
1:A:104:LEU:CD2	1:A:121:CYS:SG	0.40	3.10	18	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	143/162 (88%)	108±3 (75±2%)	26±4 (18±3%)	9±3 (7±2%)	3	19
All	All	3003/3402 (88%)	2259 (75%)	545 (18%)	199 (7%)	3	19

All 51 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	8	LYS	14
1	A	12	ILE	13
1	A	40	ARG	11
1	A	101	LYS	10
1	A	99	TYR	10
1	A	125	THR	9
1	A	128	VAL	8
1	A	126	PRO	7
1	A	7	MET	7
1	A	145	MET	7
1	A	80	ALA	5
1	A	127	GLU	5
1	A	111	ALA	5
1	A	110	SER	5
1	A	146	HIS	5
1	A	77	LYS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	130	ASP	5
1	A	9	GLY	4
1	A	89	GLU	4
1	A	33	ASP	4
1	A	6	THR	4
1	A	144	PRO	3
1	A	78	ILE	3
1	A	95	LEU	3
1	A	76	THR	3
1	A	141	LYS	2
1	A	53	ASP	2
1	A	117	LEU	2
1	A	85	ASP	2
1	A	113	PRO	2
1	A	51	GLU	2
1	A	116	SER	2
1	A	11	ASP	2
1	A	87	LEU	2
1	A	100	LYS	2
1	A	66	CYS	2
1	A	16	ALA	2
1	A	88	ASN	2
1	A	43	VAL	2
1	A	112	GLU	1
1	A	152	ASN	1
1	A	114	GLU	1
1	A	90	ASN	1
1	A	22	LEU	1
1	A	14	LYS	1
1	A	48	PRO	1
1	A	15	VAL	1
1	A	151	PHE	1
1	A	115	GLN	1
1	A	97	THR	1
1	A	79	PRO	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	127/144 (88%)	90±5 (71±4%)	37±5 (29±4%)	2	18
All	All	2667/3024 (88%)	1885 (71%)	782 (29%)	2	18

All 100 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	135	LYS	19
1	A	137	ASP	19
1	A	143	LEU	19
1	A	58	LEU	19
1	A	83	LYS	18
1	A	70	LYS	18
1	A	60	LYS	16
1	A	14	LYS	15
1	A	39	LEU	15
1	A	125	THR	15
1	A	18	THR	14
1	A	11	ASP	14
1	A	95	LEU	14
1	A	28	ASP	14
1	A	101	LYS	13
1	A	32	LEU	13
1	A	91	LYS	13
1	A	57	LEU	13
1	A	55	GLU	12
1	A	145	MET	12
1	A	77	LYS	12
1	A	116	SER	11
1	A	87	LEU	11
1	A	146	HIS	11
1	A	98	ASP	11
1	A	74	GLU	11
1	A	96	ASP	11
1	A	130	ASP	11
1	A	117	LEU	10
1	A	93	LEU	10
1	A	89	GLU	10
1	A	103	LEU	10
1	A	90	ASN	10
1	A	6	THR	9
1	A	133	LEU	9
1	A	140	LEU	9

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Mol	Chain	Res	Type	Models (Total)
1	A	124	ARG	9
1	A	75	LYS	9
1	A	30	SER	9
1	A	107	MET	8
1	A	106	CYS	8
1	A	49	THR	8
1	A	8	LYS	8
1	A	69	LYS	8
1	A	156	LEU	8
1	A	123	VAL	8
1	A	100	LYS	8
1	A	115	GLN	8
1	A	40	ARG	7
1	A	119	CYS	7
1	A	114	GLU	7
1	A	104	LEU	7
1	A	155	GLN	7
1	A	149	LEU	7
1	A	51	GLU	7
1	A	134	GLU	6
1	A	59	GLN	6
1	A	88	ASN	6
1	A	141	LYS	6
1	A	10	LEU	6
1	A	127	GLU	6
1	A	108	GLU	6
1	A	154	THR	6
1	A	110	SER	6
1	A	33	ASP	6
1	A	102	TYR	5
1	A	147	ILE	5
1	A	22	LEU	5
1	A	47	LYS	5
1	A	21	SER	4
1	A	112	GLU	4
1	A	122	LEU	4
1	A	151	PHE	4
1	A	45	GLU	4
1	A	150	SER	4
1	A	148	ARG	4
1	A	131	GLU	4
1	A	76	THR	4

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Mol	Chain	Res	Type	Models (Total)
1	A	152	ASN	3
1	A	13	GLN	3
1	A	15	VAL	3
1	A	42	TYR	3
1	A	120	GLN	3
1	A	109	ASN	3
1	A	138	LYS	3
1	A	27	SER	3
1	A	68	GLN	2
1	A	53	ASP	2
1	A	66	CYS	2
1	A	97	THR	2
1	A	46	LEU	2
1	A	84	ILE	2
1	A	7	MET	2
1	A	85	ASP	2
1	A	44	GLU	2
1	A	118	VAL	1
1	A	99	TYR	1
1	A	136	PHE	1
1	A	41	VAL	1
1	A	82	PHE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided