



Full wwPDB NMR Structure Validation Report ⓘ

Aug 22, 2016 – 05:19 PM EDT

PDB ID : 5JDP
Title : E73V mutant of the human voltage-dependent anion channel
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Deposited on : 2016-04-17

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-20027939
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

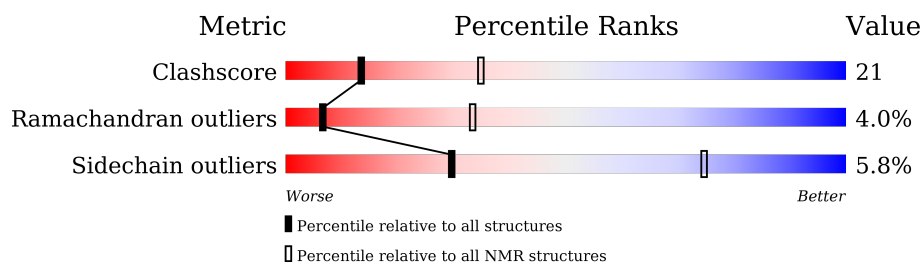
1 Overall quality at a glance

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	285	 58% 28% . 11%

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models).

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:2-A:18, A:24-A:89, A:93-A:103, A:109-A:197, A:202-A:211, A:216-A:250, A:254-A:265, A:271-A:283 (253)	0.55	4

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

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

The models can be grouped into 3 clusters and 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4346 atoms, of which 2162 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Voltage-dependent anion-selective channel protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	285	Total	C	H	N	O	S	0
			4346	1379	2162	371	430	4	

There are 4 discrepancies between the modelled and reference sequences:

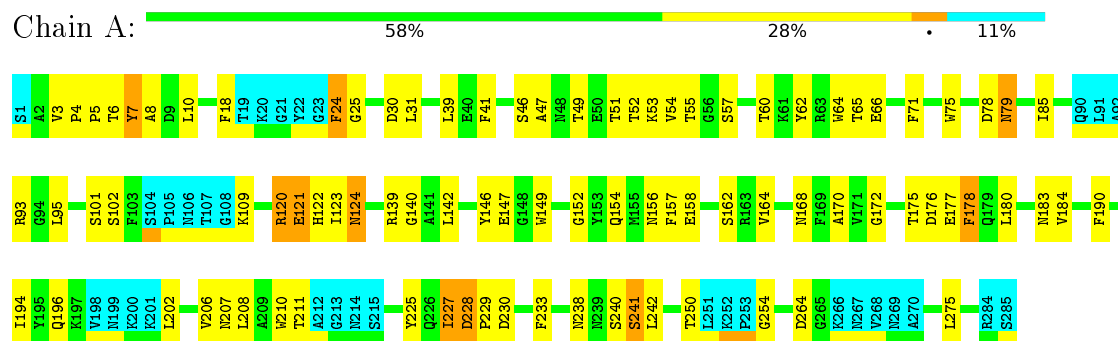
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P21796
A	73	VAL	GLU	conflict	UNP P21796
A	284	ARG	-	expression tag	UNP P21796
A	285	SER	-	expression tag	UNP P21796

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: Voltage-dependent anion-selective channel protein 1

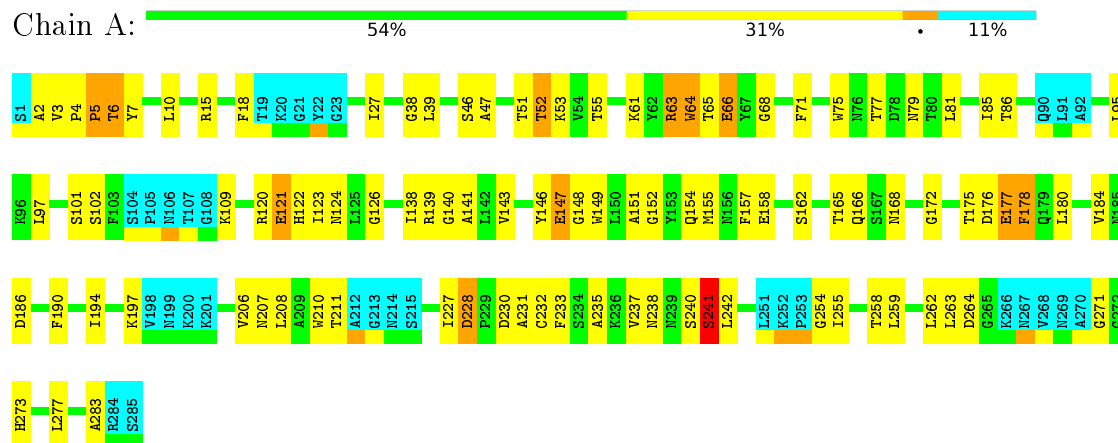


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

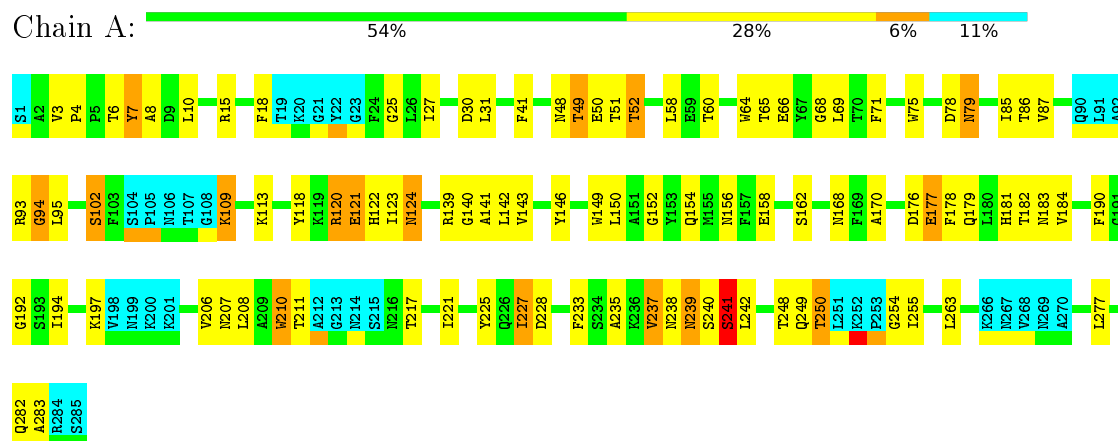
4.2.1 Score per residue for model 1

- Molecule 1: Voltage-dependent anion-selective channel protein 1



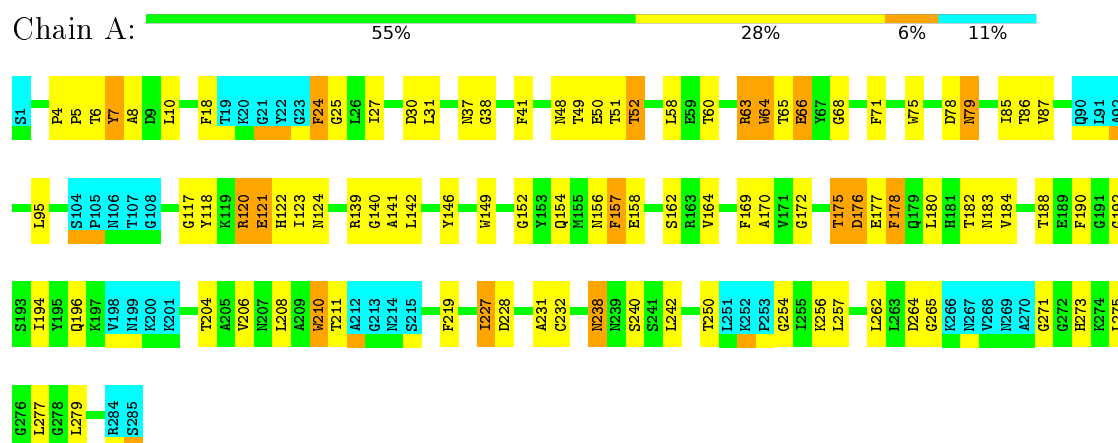
4.2.2 Score per residue for model 2

- Molecule 1: Voltage-dependent anion-selective channel protein 1



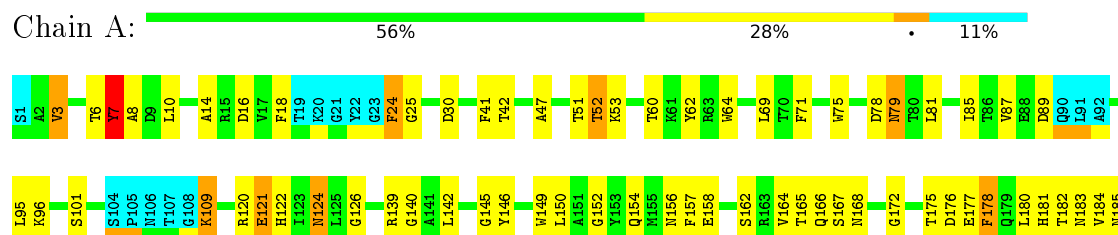
4.2.3 Score per residue for model 3

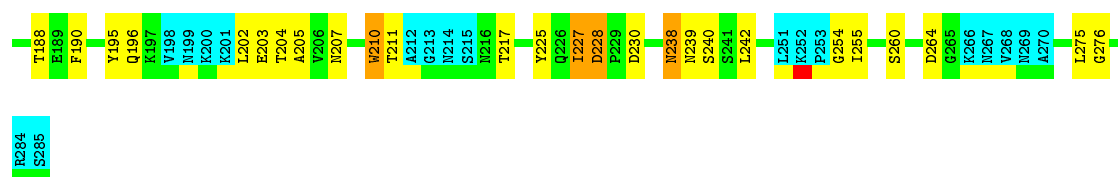
- Molecule 1: Voltage-dependent anion-selective channel protein 1



4.2.4 Score per residue for model 4 (medoid)

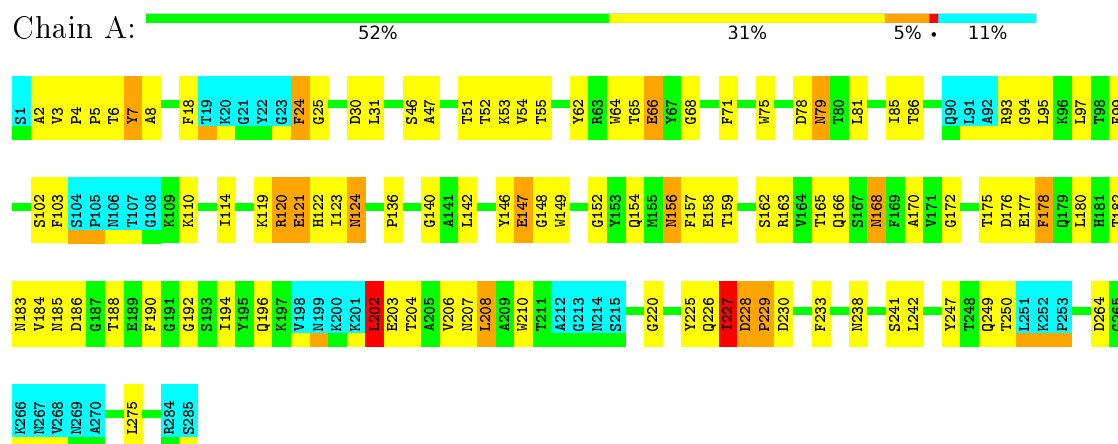
- Molecule 1: Voltage-dependent anion-selective channel protein 1





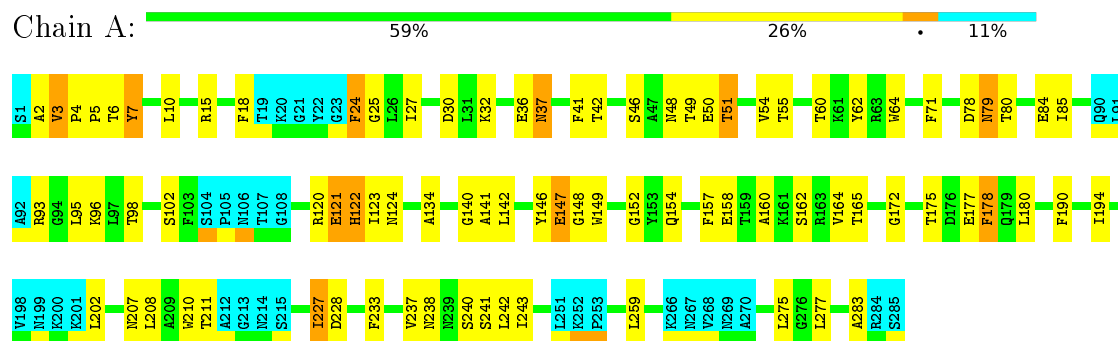
4.2.5 Score per residue for model 5

- Molecule 1: Voltage-dependent anion-selective channel protein 1



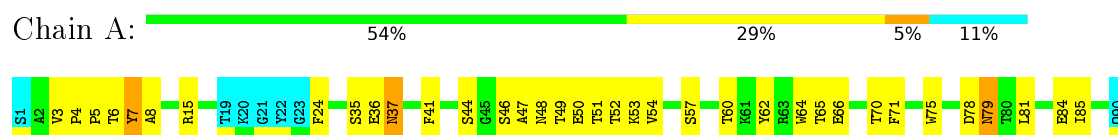
4.2.6 Score per residue for model 6

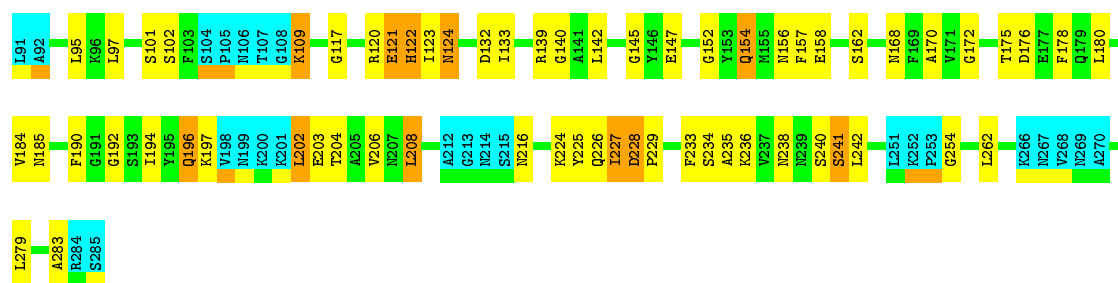
- Molecule 1: Voltage-dependent anion-selective channel protein 1



4.2.7 Score per residue for model 7

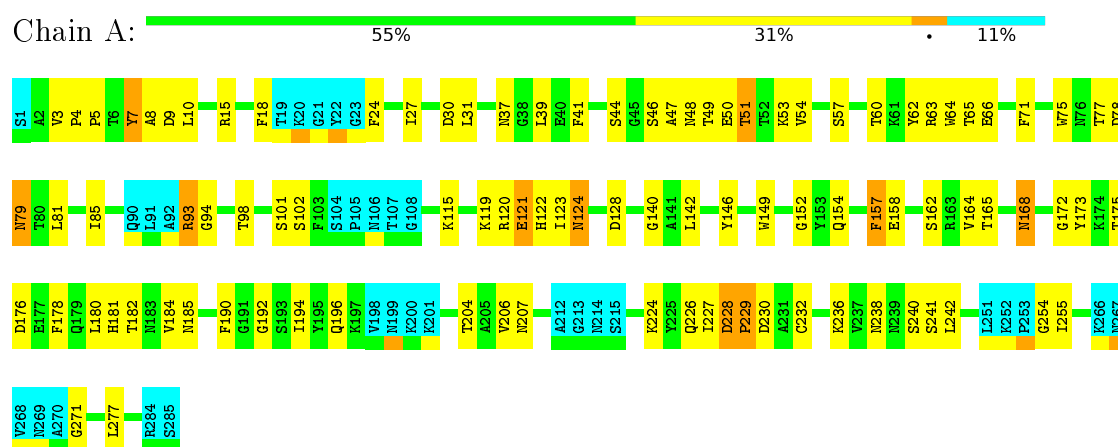
- Molecule 1: Voltage-dependent anion-selective channel protein 1





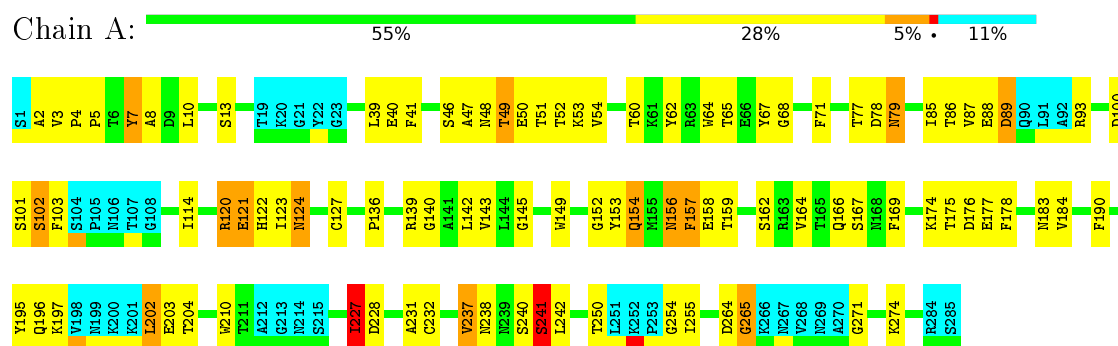
4.2.8 Score per residue for model 8

- Molecule 1: Voltage-dependent anion-selective channel protein 1



4.2.9 Score per residue for model 9

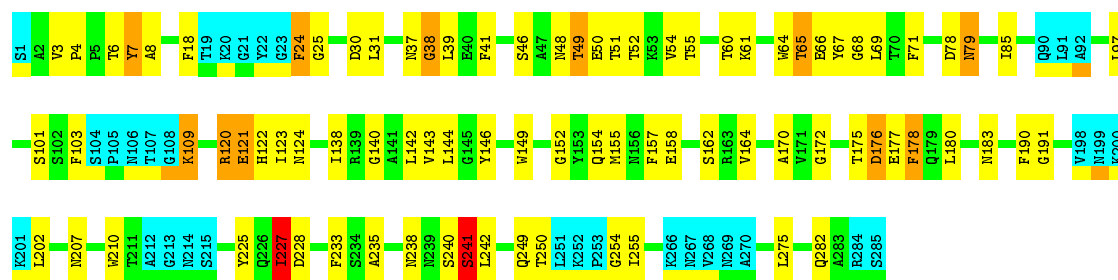
- Molecule 1: Voltage-dependent anion-selective channel protein 1



4.2.10 Score per residue for model 10

- Molecule 1: Voltage-dependent anion-selective channel protein 1

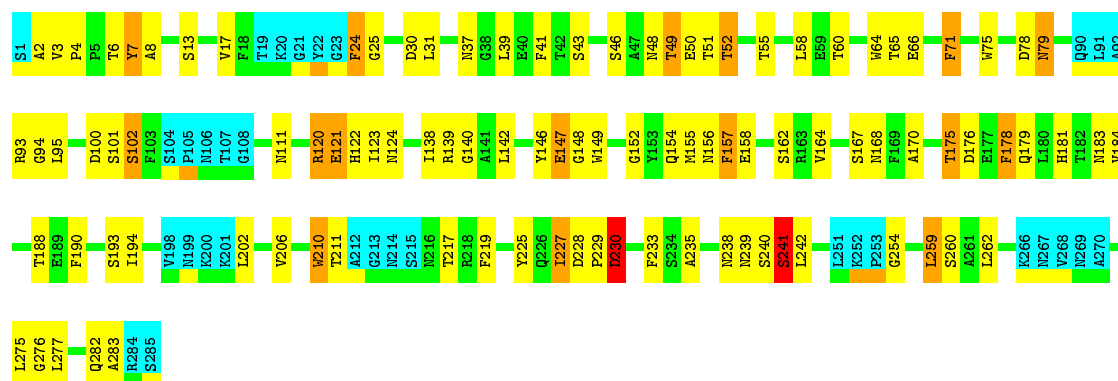




4.2.11 Score per residue for model 11

- Molecule 1: Voltage-dependent anion-selective channel protein 1

Chain A: 53% 29% 6% 11%



4.2.12 Score per residue for model 12

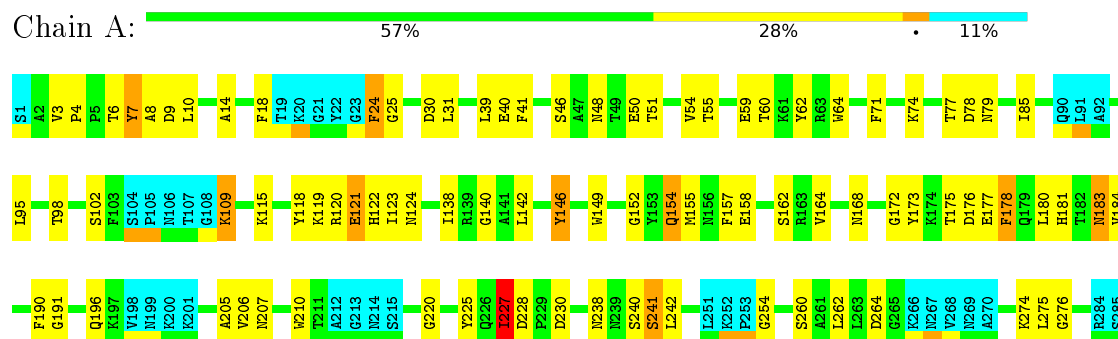
- Molecule 1: Voltage-dependent anion-selective channel protein 1

Chain A: 51% 31% 6% 11%



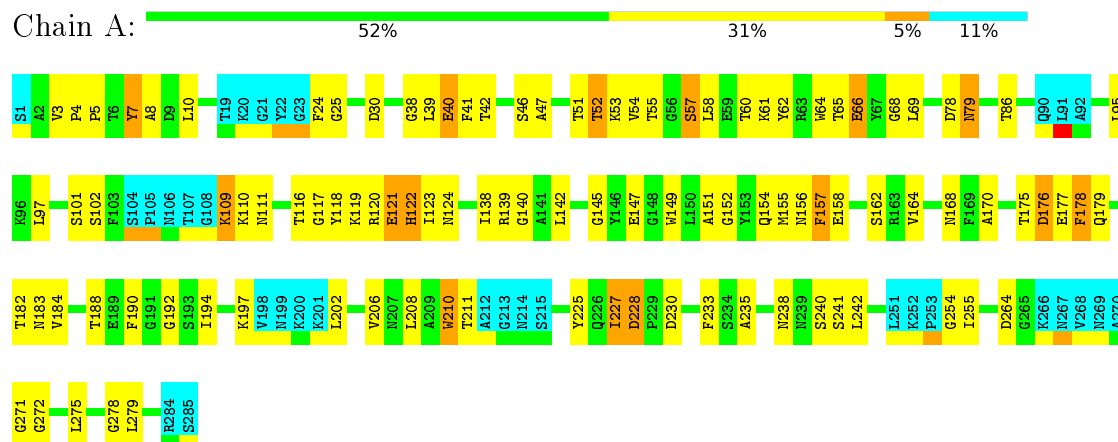
4.2.13 Score per residue for model 13

- Molecule 1: Voltage-dependent anion-selective channel protein 1



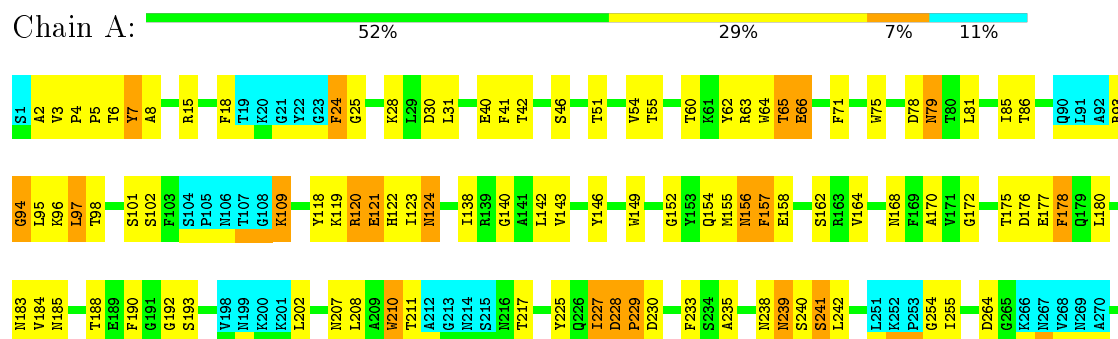
4.2.14 Score per residue for model 14

- Molecule 1: Voltage-dependent anion-selective channel protein 1



4.2.15 Score per residue for model 15

- Molecule 1: Voltage-dependent anion-selective channel protein 1

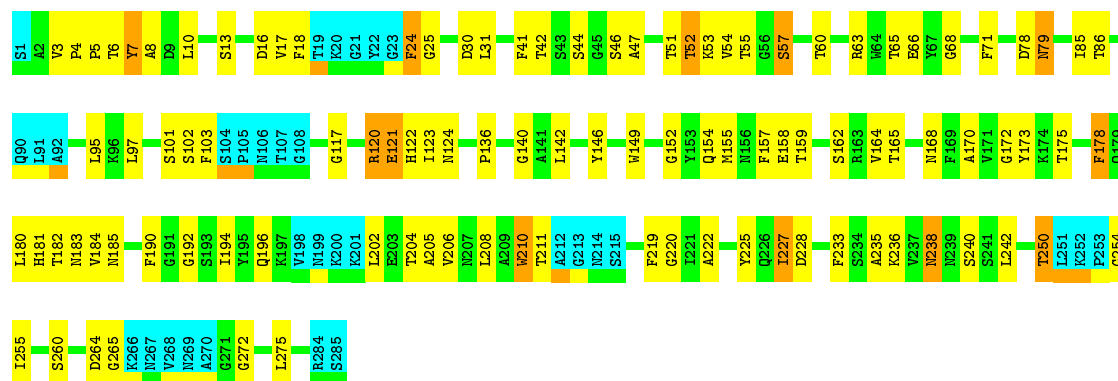




4.2.16 Score per residue for model 16

- Molecule 1: Voltage-dependent anion-selective channel protein 1

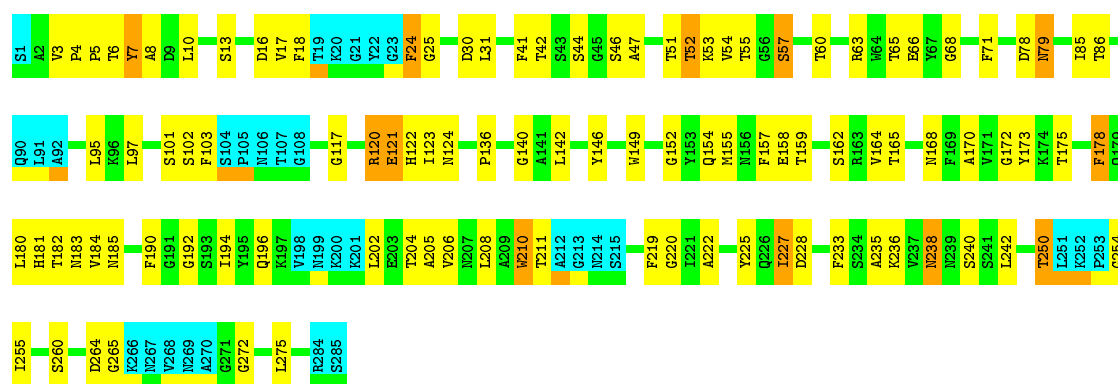
Chain A:  52% 32% . 11%



4.2.17 Score per residue for model 17

- Molecule 1: Voltage-dependent anion-selective channel protein 1

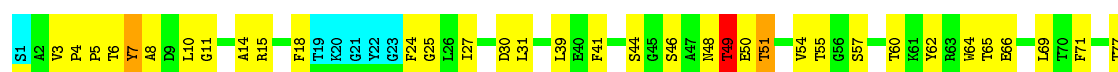
Chain A:  52% 32% • 11%

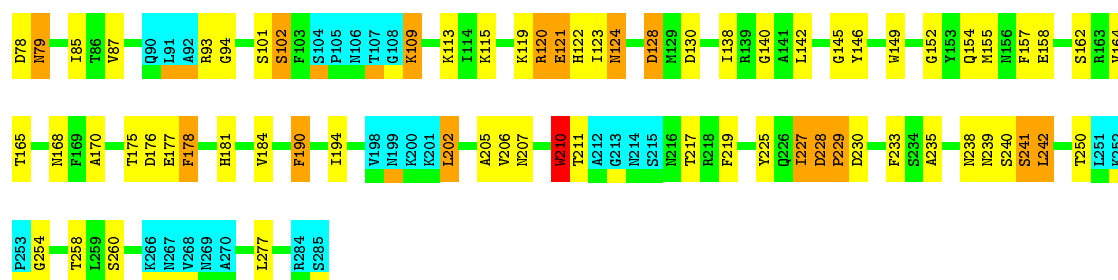


4.2.18 Score per residue for model 18

- Molecule 1: Voltage-dependent anion-selective channel protein 1

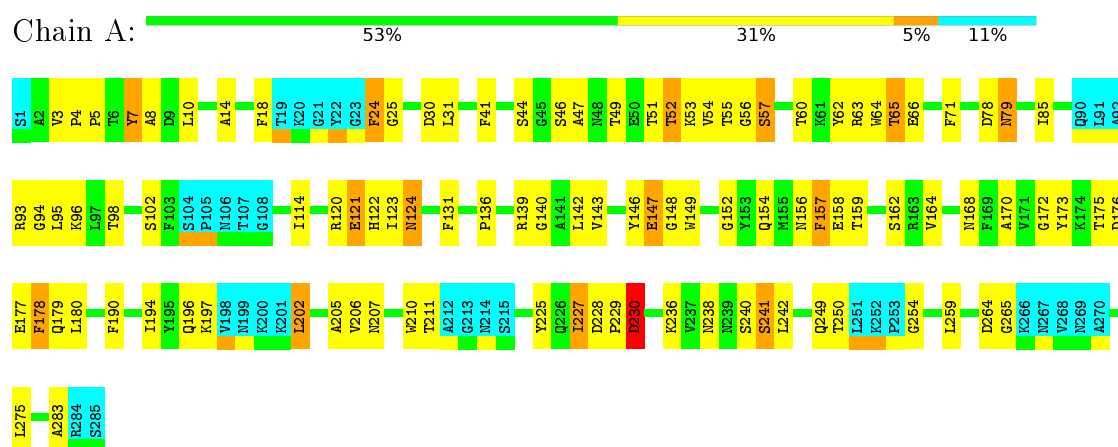
Chain A: 53% 29% 6% 11%





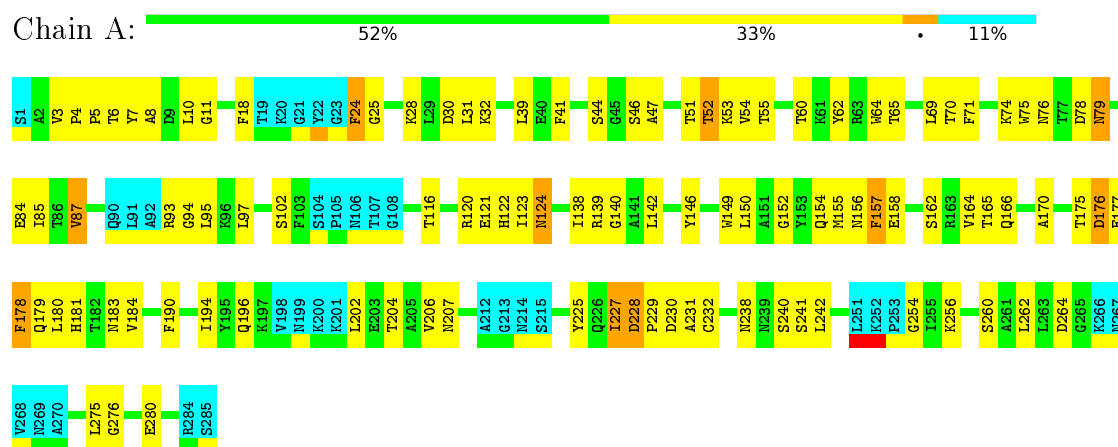
4.2.19 Score per residue for model 19

- Molecule 1: Voltage-dependent anion-selective channel protein 1



4.2.20 Score per residue for model 20

- Molecule 1: Voltage-dependent anion-selective channel protein 1



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 20 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR NIH	refinement	

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

Chemical shift file(s)	5jdp_cs.cif
Number of chemical shift lists	1
Total number of shifts	971
Number of shifts mapped to atoms	0
Number of unparsed shifts	971
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.69±0.01	0±0/1992 (0.0±0.0%)	0.88±0.01	1±1/2694 (0.0±0.0%)
All	All	0.69	0/39840 (0.0%)	0.88	23/53880 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	227	ILE	CA-CB-CG1	7.61	125.45	111.00	20	3
1	A	227	ILE	CA-CB-CG2	6.56	124.02	110.90	1	3
1	A	227	ILE	CB-CA-C	6.56	124.72	111.60	9	10
1	A	227	ILE	CG1-CB-CG2	6.48	125.65	111.40	6	4
1	A	227	ILE	CB-CG1-CD1	-5.49	98.52	113.90	13	2
1	A	210	TRP	CD1-NE1-CE2	5.03	113.53	109.00	18	1

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	1953	1920	1920	81±9
All	All	39060	38400	38400	1627

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:238:ASN:ND2	1:A:242:LEU:H	0.92	1.60	3	4
1:A:238:ASN:HD21	1:A:242:LEU:H	0.79	1.20	3	4
1:A:259:LEU:HD22	1:A:259:LEU:N	0.77	1.93	11	1
1:A:63:ARG:O	1:A:64:TRP:CG	0.77	2.38	1	2
1:A:238:ASN:HD21	1:A:242:LEU:HD13	0.77	1.39	10	7
1:A:259:LEU:N	1:A:259:LEU:HD22	0.76	1.95	6	1
1:A:178:PHE:CE1	1:A:194:ILE:HG23	0.76	2.15	19	1
1:A:2:ALA:O	1:A:3:VAL:HG13	0.76	1.80	6	4
1:A:175:THR:HG21	1:A:178:PHE:CE1	0.74	2.17	9	1
1:A:146:TYR:O	1:A:148:GLY:N	0.73	2.21	5	6
1:A:7:TYR:CG	1:A:8:ALA:N	0.72	2.57	20	18
1:A:149:TRP:N	1:A:149:TRP:CD1	0.72	2.56	13	7
1:A:46:SER:O	1:A:54:VAL:HG13	0.70	1.86	18	3
1:A:149:TRP:CD1	1:A:149:TRP:N	0.70	2.59	10	9
1:A:5:PRO:O	1:A:124:ASN:ND2	0.69	2.24	6	2
1:A:7:TYR:CD2	1:A:8:ALA:N	0.68	2.61	4	9
1:A:10:LEU:HD11	1:A:181:HIS:CE1	0.67	2.24	4	2
1:A:87:VAL:O	1:A:87:VAL:HG23	0.67	1.90	2	1
1:A:242:LEU:N	1:A:242:LEU:HD12	0.66	2.05	8	3
1:A:114:ILE:HD12	1:A:131:PHE:CE2	0.66	2.25	19	1
1:A:184:VAL:HG13	1:A:190:PHE:CE2	0.66	2.25	2	7
1:A:10:LEU:HD23	1:A:150:LEU:HD13	0.66	1.67	2	1
1:A:210:TRP:CG	1:A:211:THR:N	0.66	2.64	3	7
1:A:142:LEU:O	1:A:152:GLY:HA2	0.66	1.91	20	19
1:A:10:LEU:HD21	1:A:181:HIS:CE1	0.66	2.25	16	2
1:A:5:PRO:O	1:A:6:THR:HG23	0.65	1.90	1	2
1:A:146:TYR:O	1:A:149:TRP:CD1	0.64	2.50	18	10
1:A:120:ARG:O	1:A:121:GLU:O	0.64	2.15	1	15
1:A:140:GLY:O	1:A:154:GLN:HA	0.64	1.92	13	19
1:A:62:TYR:CZ	1:A:64:TRP:CD1	0.64	2.86	5	2
1:A:18:PHE:CG	1:A:207:ASN:ND2	0.64	2.65	6	3
1:A:4:PRO:CB	1:A:10:LEU:HD11	0.64	2.23	19	2
1:A:228:ASP:N	1:A:229:PRO:CD	0.64	2.61	5	2
1:A:183:ASN:OD1	1:A:184:VAL:N	0.64	2.31	9	3
1:A:219:PHE:CE2	1:A:239:ASN:ND2	0.64	2.66	18	2
1:A:74:LYS:NZ	1:A:76:ASN:ND2	0.64	2.46	20	1
1:A:202:LEU:HD21	1:A:225:TYR:CE2	0.63	2.29	4	2
1:A:238:ASN:OD1	1:A:242:LEU:N	0.63	2.30	5	9
1:A:124:ASN:HD22	1:A:143:VAL:HG21	0.63	1.53	9	2
1:A:210:TRP:NE1	1:A:217:THR:OG1	0.63	2.31	18	1
1:A:87:VAL:HG13	1:A:87:VAL:O	0.63	1.94	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:238:ASN:C	1:A:238:ASN:HD22	0.63	1.97	4	2
1:A:178:PHE:CD1	1:A:196:GLN:NE2	0.62	2.67	12	1
1:A:175:THR:OG1	1:A:178:PHE:N	0.62	2.32	13	7
1:A:271:GLY:O	1:A:273:HIS:CE1	0.62	2.52	1	1
1:A:6:THR:HG22	1:A:141:ALA:HB3	0.62	1.71	3	2
1:A:5:PRO:N	1:A:119:LYS:HZ1	0.62	1.92	18	1
1:A:149:TRP:C	1:A:150:LEU:HD12	0.62	2.14	4	1
1:A:190:PHE:CD2	1:A:210:TRP:NE1	0.62	2.68	6	5
1:A:93:ARG:O	1:A:95:LEU:N	0.62	2.33	20	6
1:A:225:TYR:CE2	1:A:227:ILE:HB	0.62	2.30	16	5
1:A:178:PHE:CD1	1:A:178:PHE:N	0.62	2.67	12	2
1:A:71:PHE:CD2	1:A:85:ILE:HG23	0.61	2.30	10	5
1:A:184:VAL:HG13	1:A:190:PHE:CE1	0.61	2.30	7	8
1:A:238:ASN:ND2	1:A:242:LEU:HD13	0.61	2.09	7	5
1:A:4:PRO:O	1:A:124:ASN:ND2	0.61	2.34	9	5
1:A:7:TYR:CD1	1:A:8:ALA:N	0.61	2.68	8	4
1:A:87:VAL:O	1:A:87:VAL:HG13	0.61	1.95	9	1
1:A:178:PHE:CE2	1:A:194:ILE:HG23	0.61	2.31	2	2
1:A:62:TYR:CE1	1:A:64:TRP:NE1	0.61	2.68	9	7
1:A:233:PHE:CZ	1:A:235:ALA:HB2	0.61	2.31	16	10
1:A:190:PHE:CE1	1:A:210:TRP:CZ2	0.61	2.89	16	2
1:A:175:THR:O	1:A:177:GLU:N	0.61	2.34	10	9
1:A:62:TYR:CE2	1:A:64:TRP:NE1	0.61	2.69	7	6
1:A:7:TYR:CD2	1:A:7:TYR:C	0.61	2.74	10	5
1:A:249:GLN:O	1:A:250:THR:OG1	0.61	2.17	10	2
1:A:7:TYR:CD1	1:A:7:TYR:C	0.60	2.75	2	6
1:A:64:TRP:O	1:A:66:GLU:N	0.60	2.34	5	8
1:A:38:GLY:O	1:A:61:LYS:O	0.60	2.20	14	4
1:A:217:THR:O	1:A:239:ASN:ND2	0.60	2.35	4	2
1:A:139:ARG:NH1	1:A:156:ASN:ND2	0.60	2.50	20	1
1:A:190:PHE:CD1	1:A:210:TRP:NE1	0.60	2.69	12	3
1:A:238:ASN:HD22	1:A:238:ASN:C	0.60	1.98	3	2
1:A:238:ASN:ND2	1:A:240:SER:OG	0.60	2.35	8	7
1:A:238:ASN:OD1	1:A:242:LEU:HD12	0.60	1.97	3	2
1:A:7:TYR:CZ	1:A:183:ASN:ND2	0.60	2.69	3	2
1:A:71:PHE:CD1	1:A:85:ILE:HG23	0.60	2.31	16	5
1:A:227:ILE:HB	1:A:229:PRO:HD2	0.60	1.71	18	2
1:A:3:VAL:O	1:A:3:VAL:HG23	0.60	1.95	2	2
1:A:139:ARG:HE	1:A:156:ASN:ND2	0.60	1.95	19	4
1:A:3:VAL:HG13	1:A:3:VAL:O	0.60	1.95	9	2
1:A:95:LEU:HD23	1:A:96:LYS:N	0.60	2.12	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:VAL:O	1:A:3:VAL:HG13	0.59	1.96	13	1
1:A:75:TRP:CE2	1:A:81:LEU:HD22	0.59	2.32	4	4
1:A:7:TYR:H	1:A:141:ALA:CB	0.59	2.11	1	2
1:A:7:TYR:CD2	1:A:170:ALA:HB2	0.59	2.33	12	7
1:A:276:GLY:C	1:A:277:LEU:HD12	0.59	2.18	12	3
1:A:173:TYR:CD1	1:A:173:TYR:N	0.59	2.70	19	1
1:A:69:LEU:CD2	1:A:87:VAL:HG22	0.59	2.28	4	2
1:A:206:VAL:HG13	1:A:220:GLY:O	0.59	1.98	5	3
1:A:259:LEU:CD2	1:A:259:LEU:N	0.59	2.66	11	2
1:A:210:TRP:CD1	1:A:211:THR:N	0.58	2.71	3	1
1:A:158:GLU:O	1:A:162:SER:N	0.58	2.37	11	20
1:A:156:ASN:HD22	1:A:156:ASN:N	0.58	1.94	15	1
1:A:184:VAL:HG13	1:A:190:PHE:CZ	0.58	2.33	7	6
1:A:32:LYS:NZ	1:A:256:LYS:NZ	0.58	2.51	20	1
1:A:139:ARG:NE	1:A:156:ASN:ND2	0.58	2.52	7	2
1:A:75:TRP:CE2	1:A:81:LEU:CD2	0.58	2.87	5	2
1:A:140:GLY:O	1:A:154:GLN:NE2	0.58	2.37	5	4
1:A:39:LEU:HD22	1:A:41:PHE:CE1	0.58	2.34	11	3
1:A:9:ASP:OD1	1:A:115:LYS:NZ	0.57	2.37	12	1
1:A:6:THR:HG23	1:A:124:ASN:ND2	0.57	2.14	1	1
1:A:124:ASN:HD22	1:A:143:VAL:CG2	0.57	2.11	9	2
1:A:238:ASN:HD21	1:A:242:LEU:N	0.57	1.97	4	2
1:A:122:HIS:ND1	1:A:122:HIS:C	0.57	2.57	4	1
1:A:3:VAL:O	1:A:5:PRO:HD3	0.57	1.99	1	1
1:A:202:LEU:CD1	1:A:203:GLU:H	0.57	2.13	5	1
1:A:32:LYS:O	1:A:283:ALA:HB3	0.57	2.00	6	1
1:A:2:ALA:HB2	1:A:174:LYS:NZ	0.57	2.14	9	1
1:A:176:ASP:O	1:A:178:PHE:CG	0.57	2.58	7	3
1:A:48:ASN:O	1:A:51:THR:N	0.57	2.38	18	4
1:A:190:PHE:CD2	1:A:190:PHE:N	0.57	2.72	17	6
1:A:190:PHE:N	1:A:190:PHE:CD2	0.57	2.72	16	5
1:A:48:ASN:O	1:A:50:GLU:N	0.57	2.38	7	7
1:A:7:TYR:CE1	1:A:183:ASN:ND2	0.57	2.73	20	2
1:A:190:PHE:N	1:A:190:PHE:CD1	0.56	2.73	4	3
1:A:242:LEU:HD12	1:A:242:LEU:N	0.56	2.15	19	4
1:A:7:TYR:OH	1:A:168:ASN:ND2	0.56	2.39	2	5
1:A:147:GLU:O	1:A:149:TRP:NE1	0.56	2.39	5	5
1:A:227:ILE:HG22	1:A:228:ASP:N	0.56	2.15	4	2
1:A:142:LEU:N	1:A:142:LEU:HD12	0.56	2.15	16	2
1:A:142:LEU:HD12	1:A:142:LEU:N	0.56	2.15	17	1
1:A:202:LEU:HD11	1:A:225:TYR:CD1	0.56	2.35	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:194:ILE:HD11	1:A:208:LEU:HD11	0.56	1.78	1	2
1:A:178:PHE:CD2	1:A:178:PHE:N	0.56	2.71	5	2
1:A:121:GLU:O	1:A:123:ILE:N	0.56	2.39	15	19
1:A:24:PHE:CD2	1:A:260:SER:OG	0.56	2.59	16	2
1:A:71:PHE:CE2	1:A:85:ILE:HG23	0.55	2.36	6	8
1:A:44:SER:OG	1:A:57:SER:N	0.55	2.40	18	5
1:A:168:ASN:N	1:A:168:ASN:OD1	0.55	2.39	5	1
1:A:96:LYS:NZ	1:A:98:THR:OG1	0.55	2.38	15	3
1:A:192:GLY:N	1:A:208:LEU:O	0.55	2.40	7	9
1:A:157:PHE:CE2	1:A:164:VAL:CG2	0.55	2.90	11	3
1:A:7:TYR:C	1:A:7:TYR:CD2	0.55	2.79	12	4
1:A:190:PHE:CD1	1:A:190:PHE:N	0.55	2.73	14	4
1:A:24:PHE:CB	1:A:260:SER:HG	0.55	2.13	18	1
1:A:95:LEU:C	1:A:95:LEU:HD23	0.55	2.21	6	1
1:A:140:GLY:N	1:A:154:GLN:HE22	0.55	1.99	16	3
1:A:124:ASN:N	1:A:124:ASN:OD1	0.55	2.39	2	1
1:A:9:ASP:OD2	1:A:115:LYS:NZ	0.55	2.40	13	2
1:A:13:SER:O	1:A:17:VAL:HG23	0.54	2.02	16	3
1:A:282:GLN:O	1:A:283:ALA:HB3	0.54	2.01	11	2
1:A:156:ASN:OD1	1:A:156:ASN:N	0.54	2.38	9	1
1:A:7:TYR:C	1:A:7:TYR:CD1	0.54	2.78	17	1
1:A:203:GLU:O	1:A:204:THR:HG23	0.54	2.01	12	3
1:A:39:LEU:HD22	1:A:41:PHE:CE2	0.54	2.38	13	3
1:A:150:LEU:N	1:A:150:LEU:HD12	0.54	2.18	4	1
1:A:118:TYR:CZ	1:A:119:LYS:O	0.54	2.60	14	2
1:A:124:ASN:ND2	1:A:143:VAL:HG21	0.54	2.16	19	2
1:A:118:TYR:CE2	1:A:119:LYS:O	0.54	2.61	14	1
1:A:7:TYR:CE1	1:A:168:ASN:ND2	0.54	2.75	1	1
1:A:18:PHE:CD1	1:A:207:ASN:ND2	0.54	2.76	18	2
1:A:143:VAL:C	1:A:144:LEU:HD22	0.54	2.23	10	1
1:A:156:ASN:ND2	1:A:156:ASN:N	0.54	2.52	15	1
1:A:194:ILE:HD12	1:A:206:VAL:HB	0.54	1.80	2	14
1:A:30:ASP:OD2	1:A:31:LEU:N	0.54	2.41	8	8
1:A:25:GLY:O	1:A:49:THR:HG23	0.54	2.03	11	4
1:A:4:PRO:HB2	1:A:10:LEU:HD11	0.54	1.79	19	2
1:A:51:THR:C	1:A:52:THR:HG23	0.54	2.22	10	2
1:A:10:LEU:HD23	1:A:11:GLY:N	0.54	2.18	18	2
1:A:157:PHE:CE1	1:A:164:VAL:CG2	0.54	2.91	13	7
1:A:172:GLY:HA2	1:A:180:LEU:O	0.54	2.03	8	13
1:A:103:PHE:CD2	1:A:103:PHE:N	0.54	2.75	9	1
1:A:4:PRO:O	1:A:124:ASN:CB	0.53	2.56	3	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:LYS:HZ2	1:A:256:LYS:NZ	0.53	1.99	20	1
1:A:30:ASP:OD1	1:A:31:LEU:N	0.53	2.40	11	6
1:A:146:TYR:O	1:A:149:TRP:HD1	0.53	1.86	16	3
1:A:272:GLY:O	1:A:273:HIS:CD2	0.53	2.61	12	1
1:A:62:TYR:CE1	1:A:64:TRP:CD1	0.53	2.96	9	5
1:A:228:ASP:OD1	1:A:230:ASP:N	0.53	2.42	14	2
1:A:64:TRP:C	1:A:66:GLU:H	0.53	2.06	10	7
1:A:238:ASN:ND2	1:A:242:LEU:N	0.53	2.46	4	2
1:A:158:GLU:OE1	1:A:158:GLU:N	0.53	2.41	5	1
1:A:115:LYS:NZ	1:A:128:ASP:OD1	0.53	2.41	18	1
1:A:142:LEU:O	1:A:152:GLY:CA	0.53	2.56	9	8
1:A:168:ASN:ND2	1:A:183:ASN:ND2	0.53	2.57	15	1
1:A:94:GLY:O	1:A:118:TYR:CD1	0.53	2.61	15	1
1:A:44:SER:HG	1:A:57:SER:CB	0.53	2.16	19	1
1:A:225:TYR:CZ	1:A:227:ILE:HB	0.53	2.37	2	4
1:A:3:VAL:O	1:A:124:ASN:ND2	0.53	2.42	11	1
1:A:226:GLN:NE2	1:A:228:ASP:O	0.53	2.41	12	1
1:A:14:ALA:HB1	1:A:205:ALA:HB1	0.53	1.80	4	4
1:A:183:ASN:ND2	1:A:191:GLY:O	0.53	2.42	10	1
1:A:99:PHE:CE1	1:A:114:ILE:HG23	0.53	2.39	5	1
1:A:139:ARG:NH2	1:A:156:ASN:ND2	0.53	2.57	9	1
1:A:178:PHE:N	1:A:178:PHE:CD2	0.52	2.77	3	2
1:A:254:GLY:N	1:A:282:GLN:OE1	0.52	2.41	10	1
1:A:210:TRP:C	1:A:210:TRP:CD1	0.52	2.82	16	5
1:A:210:TRP:CD1	1:A:210:TRP:C	0.52	2.82	17	4
1:A:202:LEU:HD12	1:A:203:GLU:H	0.52	1.64	5	1
1:A:63:ARG:O	1:A:65:THR:N	0.52	2.42	15	4
1:A:18:PHE:CB	1:A:207:ASN:ND2	0.52	2.73	18	9
1:A:178:PHE:CZ	1:A:196:GLN:CD	0.52	2.82	8	1
1:A:219:PHE:CZ	1:A:239:ASN:OD1	0.52	2.62	12	2
1:A:7:TYR:CD1	1:A:170:ALA:HB2	0.52	2.39	2	7
1:A:4:PRO:O	1:A:124:ASN:CG	0.52	2.48	8	13
1:A:69:LEU:CD2	1:A:87:VAL:HG12	0.52	2.33	20	2
1:A:6:THR:O	1:A:10:LEU:N	0.52	2.43	6	2
1:A:122:HIS:CD2	1:A:145:GLY:O	0.52	2.62	4	1
1:A:7:TYR:CD2	1:A:154:GLN:OE1	0.52	2.63	6	1
1:A:202:LEU:HG	1:A:203:GLU:N	0.52	2.19	7	2
1:A:25:GLY:H	1:A:275:LEU:C	0.52	2.08	6	11
1:A:238:ASN:ND2	1:A:240:SER:H	0.52	2.02	16	4
1:A:103:PHE:CD1	1:A:103:PHE:N	0.52	2.78	17	2
1:A:103:PHE:N	1:A:103:PHE:CD1	0.52	2.78	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:238:ASN:HD21	1:A:242:LEU:CD1	0.52	2.16	10	8
1:A:27:ILE:HG23	1:A:277:LEU:HB2	0.52	1.81	18	4
1:A:70:THR:O	1:A:84:GLU:O	0.52	2.28	7	2
1:A:113:LYS:NZ	1:A:130:ASP:OD1	0.52	2.43	18	1
1:A:219:PHE:CZ	1:A:239:ASN:ND2	0.51	2.78	18	2
1:A:183:ASN:O	1:A:183:ASN:ND2	0.51	2.42	13	1
1:A:264:ASP:H	1:A:273:HIS:CE1	0.51	2.23	1	1
1:A:190:PHE:CD1	1:A:210:TRP:CZ2	0.51	2.97	9	4
1:A:241:SER:C	1:A:242:LEU:HD12	0.51	2.25	19	5
1:A:7:TYR:CE2	1:A:8:ALA:HB2	0.51	2.40	4	1
1:A:122:HIS:ND1	1:A:145:GLY:O	0.51	2.42	7	1
1:A:242:LEU:N	1:A:242:LEU:CD1	0.51	2.74	8	2
1:A:230:ASP:N	1:A:230:ASP:OD2	0.51	2.41	15	1
1:A:44:SER:OG	1:A:57:SER:CB	0.51	2.58	19	3
1:A:176:ASP:C	1:A:178:PHE:H	0.51	2.09	1	5
1:A:124:ASN:ND2	1:A:143:VAL:HG11	0.51	2.19	2	1
1:A:257:LEU:HD23	1:A:279:LEU:CD2	0.51	2.36	3	1
1:A:69:LEU:HD23	1:A:87:VAL:HG22	0.51	1.82	12	2
1:A:7:TYR:OH	1:A:183:ASN:ND2	0.51	2.44	15	3
1:A:71:PHE:CE1	1:A:85:ILE:HG23	0.51	2.40	12	8
1:A:25:GLY:CA	1:A:275:LEU:O	0.51	2.59	15	13
1:A:124:ASN:C	1:A:124:ASN:ND2	0.51	2.64	8	1
1:A:190:PHE:CG	1:A:210:TRP:CE2	0.51	2.99	6	5
1:A:195:TYR:CZ	1:A:203:GLU:OE1	0.51	2.63	4	1
1:A:124:ASN:ND2	1:A:143:VAL:CG2	0.51	2.74	9	2
1:A:238:ASN:C	1:A:238:ASN:ND2	0.51	2.64	3	2
1:A:35:SER:O	1:A:37:ASN:N	0.51	2.44	7	1
1:A:18:PHE:CG	1:A:207:ASN:OD1	0.51	2.64	10	1
1:A:50:GLU:C	1:A:51:THR:HG23	0.51	2.24	13	1
1:A:71:PHE:CZ	1:A:85:ILE:HG23	0.51	2.41	3	4
1:A:219:PHE:CZ	1:A:239:ASN:CG	0.51	2.84	18	2
1:A:157:PHE:CZ	1:A:164:VAL:CG2	0.51	2.93	19	1
1:A:150:LEU:N	1:A:150:LEU:CD1	0.51	2.74	4	1
1:A:227:ILE:HG23	1:A:231:ALA:HB3	0.51	1.83	9	1
1:A:51:THR:O	1:A:52:THR:CB	0.51	2.59	19	8
1:A:249:GLN:O	1:A:250:THR:CB	0.51	2.58	2	1
1:A:75:TRP:CD2	1:A:81:LEU:HD22	0.51	2.40	7	2
1:A:178:PHE:CD1	1:A:196:GLN:CD	0.51	2.84	12	2
1:A:48:ASN:ND2	1:A:51:THR:OG1	0.51	2.44	11	1
1:A:118:TYR:CE1	1:A:119:LYS:O	0.51	2.64	13	1
1:A:10:LEU:CD1	1:A:10:LEU:N	0.50	2.74	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:190:PHE:CG	1:A:210:TRP:NE1	0.50	2.79	6	1
1:A:78:ASP:O	1:A:79:ASN:ND2	0.50	2.44	5	6
1:A:228:ASP:OD2	1:A:230:ASP:N	0.50	2.44	4	1
1:A:173:TYR:HB2	1:A:180:LEU:HD12	0.50	1.82	13	3
1:A:65:THR:O	1:A:65:THR:HG22	0.50	2.05	20	1
1:A:157:PHE:CD1	1:A:164:VAL:HG22	0.50	2.42	13	3
1:A:78:ASP:O	1:A:79:ASN:CB	0.50	2.60	7	19
1:A:182:THR:HG22	1:A:192:GLY:HA2	0.50	1.83	3	7
1:A:122:HIS:O	1:A:122:HIS:ND1	0.50	2.45	4	1
1:A:238:ASN:ND2	1:A:238:ASN:C	0.50	2.64	17	2
1:A:46:SER:O	1:A:55:THR:N	0.50	2.45	5	9
1:A:77:THR:O	1:A:79:ASN:ND2	0.50	2.44	8	1
1:A:4:PRO:C	1:A:119:LYS:NZ	0.50	2.65	18	1
1:A:5:PRO:CG	1:A:143:VAL:HG11	0.50	2.36	1	1
1:A:139:ARG:C	1:A:154:GLN:HE22	0.50	2.10	1	1
1:A:65:THR:O	1:A:66:GLU:O	0.50	2.29	3	2
1:A:95:LEU:HD12	1:A:117:GLY:O	0.50	2.07	7	5
1:A:164:VAL:O	1:A:165:THR:HG23	0.50	2.07	4	6
1:A:238:ASN:ND2	1:A:242:LEU:HD12	0.50	2.22	20	3
1:A:173:TYR:HB3	1:A:180:LEU:HD12	0.50	1.83	16	2
1:A:27:ILE:HG23	1:A:277:LEU:CB	0.50	2.37	18	1
1:A:260:SER:OG	1:A:276:GLY:N	0.50	2.44	20	1
1:A:226:GLN:OE1	1:A:232:CYS:SG	0.50	2.69	12	1
1:A:118:TYR:OH	1:A:120:ARG:CZ	0.50	2.60	15	1
1:A:179:GLN:OE1	1:A:181:HIS:NE2	0.50	2.44	11	2
1:A:227:ILE:O	1:A:228:ASP:CB	0.50	2.59	8	2
1:A:46:SER:O	1:A:54:VAL:HA	0.50	2.06	10	12
1:A:102:SER:OG	1:A:103:PHE:CE1	0.50	2.65	12	1
1:A:176:ASP:O	1:A:178:PHE:CD1	0.50	2.65	1	3
1:A:238:ASN:HD21	1:A:242:LEU:CG	0.50	2.19	14	3
1:A:78:ASP:OD1	1:A:78:ASP:O	0.49	2.31	5	1
1:A:94:GLY:O	1:A:118:TYR:CD2	0.49	2.65	2	1
1:A:48:ASN:C	1:A:50:GLU:H	0.49	2.11	11	4
1:A:41:PHE:CZ	1:A:60:THR:HG23	0.49	2.42	13	4
1:A:13:SER:OG	1:A:195:TYR:CD1	0.49	2.64	12	1
1:A:3:VAL:CA	1:A:124:ASN:HD21	0.49	2.20	14	1
1:A:175:THR:C	1:A:177:GLU:N	0.49	2.66	20	9
1:A:196:GLN:NE2	1:A:204:THR:OG1	0.49	2.45	8	1
1:A:184:VAL:HG22	1:A:190:PHE:CE1	0.49	2.43	1	1
1:A:5:PRO:C	1:A:6:THR:HG23	0.49	2.28	1	1
1:A:263:LEU:HD12	1:A:263:LEU:N	0.49	2.23	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:PHE:CE2	1:A:60:THR:OG1	0.49	2.63	3	9
1:A:119:LYS:CG	1:A:124:ASN:HD22	0.49	2.20	14	1
1:A:41:PHE:CE1	1:A:60:THR:OG1	0.49	2.63	8	5
1:A:50:GLU:O	1:A:51:THR:CB	0.49	2.60	8	3
1:A:124:ASN:ND2	1:A:143:VAL:CG1	0.49	2.75	2	1
1:A:87:VAL:O	1:A:87:VAL:CG2	0.49	2.61	2	1
1:A:27:ILE:HG23	1:A:277:LEU:HB3	0.49	1.84	3	2
1:A:168:ASN:ND2	1:A:185:ASN:OD1	0.49	2.45	15	3
1:A:202:LEU:CD1	1:A:203:GLU:N	0.49	2.76	5	1
1:A:40:GLU:OE1	1:A:63:ARG:NH2	0.49	2.45	15	1
1:A:17:VAL:HG12	1:A:222:ALA:HB1	0.49	1.84	16	2
1:A:5:PRO:O	1:A:6:THR:CG2	0.49	2.60	6	2
1:A:176:ASP:O	1:A:178:PHE:CD2	0.49	2.65	7	1
1:A:240:SER:OG	1:A:242:LEU:HD13	0.49	2.07	19	2
1:A:102:SER:C	1:A:103:PHE:CG	0.49	2.86	9	2
1:A:230:ASP:N	1:A:230:ASP:OD1	0.49	2.42	13	1
1:A:32:LYS:NZ	1:A:256:LYS:HZ3	0.49	2.05	20	1
1:A:157:PHE:CZ	1:A:164:VAL:HG23	0.49	2.43	9	1
1:A:57:SER:OG	1:A:58:LEU:N	0.49	2.46	14	1
1:A:58:LEU:HD12	1:A:75:TRP:CE3	0.48	2.43	3	3
1:A:6:THR:HG22	1:A:126:GLY:HA3	0.48	1.85	4	1
1:A:119:LYS:O	1:A:120:ARG:CB	0.48	2.61	15	2
1:A:48:ASN:O	1:A:52:THR:OG1	0.48	2.30	7	2
1:A:238:ASN:OD1	1:A:240:SER:OG	0.48	2.31	16	2
1:A:229:PRO:O	1:A:230:ASP:CB	0.48	2.61	19	2
1:A:168:ASN:HD21	1:A:183:ASN:ND2	0.48	2.06	15	2
1:A:5:PRO:C	1:A:124:ASN:ND2	0.48	2.67	3	4
1:A:7:TYR:CE2	1:A:183:ASN:ND2	0.48	2.81	3	1
1:A:237:VAL:HG13	1:A:243:ILE:HG12	0.48	1.85	6	1
1:A:176:ASP:O	1:A:178:PHE:N	0.48	2.46	1	4
1:A:63:ARG:O	1:A:64:TRP:CB	0.48	2.61	3	1
1:A:62:TYR:OH	1:A:64:TRP:CE2	0.48	2.65	5	1
1:A:240:SER:OG	1:A:242:LEU:CD1	0.48	2.61	13	4
1:A:149:TRP:N	1:A:149:TRP:HD1	0.48	2.04	8	4
1:A:183:ASN:C	1:A:183:ASN:ND2	0.48	2.65	13	1
1:A:64:TRP:C	1:A:66:GLU:N	0.48	2.67	5	8
1:A:63:ARG:CZ	1:A:65:THR:HG21	0.48	2.39	16	2
1:A:250:THR:OG1	1:A:255:ILE:O	0.48	2.26	10	1
1:A:154:GLN:NE2	1:A:155:MET:N	0.48	2.60	16	2
1:A:225:TYR:C	1:A:232:CYS:SG	0.48	2.92	20	1
1:A:221:ILE:HD12	1:A:237:VAL:CG1	0.48	2.38	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:LEU:HD23	1:A:95:LEU:C	0.48	2.29	2	2
1:A:242:LEU:CD2	1:A:264:ASP:OD2	0.48	2.62	3	3
1:A:202:LEU:H	1:A:202:LEU:HD12	0.48	1.68	18	1
1:A:175:THR:O	1:A:178:PHE:O	0.48	2.30	19	2
1:A:258:THR:O	1:A:277:LEU:HD23	0.48	2.08	18	1
1:A:179:GLN:O	1:A:194:ILE:HG23	0.48	2.09	20	1
1:A:39:LEU:O	1:A:61:LYS:O	0.47	2.32	12	3
1:A:196:GLN:OE1	1:A:204:THR:OG1	0.47	2.32	20	5
1:A:4:PRO:O	1:A:124:ASN:OD1	0.47	2.32	12	2
1:A:78:ASP:O	1:A:78:ASP:OD1	0.47	2.32	12	1
1:A:74:LYS:HZ3	1:A:76:ASN:ND2	0.47	2.07	20	1
1:A:233:PHE:CE1	1:A:247:TYR:CE1	0.47	3.02	5	1
1:A:8:ALA:O	1:A:15:ARG:NH2	0.47	2.47	18	1
1:A:18:PHE:O	1:A:236:LYS:NZ	0.47	2.41	19	1
1:A:258:THR:C	1:A:259:LEU:HD12	0.47	2.29	1	1
1:A:147:GLU:C	1:A:149:TRP:CD1	0.47	2.88	5	5
1:A:138:ILE:O	1:A:155:MET:O	0.47	2.32	18	8
1:A:139:ARG:NH1	1:A:156:ASN:HD21	0.47	2.06	7	1
1:A:240:SER:O	1:A:241:SER:CB	0.47	2.62	18	12
1:A:154:GLN:OE1	1:A:168:ASN:ND2	0.47	2.46	8	4
1:A:157:PHE:CD2	1:A:164:VAL:CG2	0.47	2.97	11	2
1:A:10:LEU:HD12	1:A:10:LEU:N	0.47	2.24	9	2
1:A:225:TYR:O	1:A:227:ILE:HD12	0.47	2.10	14	2
1:A:18:PHE:CB	1:A:207:ASN:OD1	0.47	2.63	10	1
1:A:25:GLY:N	1:A:275:LEU:O	0.47	2.47	15	3
1:A:242:LEU:CD1	1:A:242:LEU:N	0.47	2.77	16	4
1:A:175:THR:OG1	1:A:178:PHE:O	0.47	2.33	4	6
1:A:3:VAL:HG13	1:A:122:HIS:N	0.47	2.24	6	1
1:A:227:ILE:HG23	1:A:229:PRO:HD2	0.47	1.85	8	1
1:A:156:ASN:ND2	1:A:166:GLN:OE1	0.47	2.47	9	1
1:A:25:GLY:O	1:A:49:THR:CG2	0.47	2.63	11	1
1:A:3:VAL:C	1:A:124:ASN:ND2	0.47	2.68	11	1
1:A:177:GLU:OE1	1:A:197:LYS:O	0.47	2.32	14	1
1:A:10:LEU:HD22	1:A:181:HIS:CE1	0.47	2.45	20	2
1:A:157:PHE:CD1	1:A:164:VAL:CG2	0.47	2.97	12	4
1:A:97:LEU:C	1:A:97:LEU:CD1	0.47	2.83	15	1
1:A:139:ARG:CZ	1:A:156:ASN:HD21	0.47	2.23	7	1
1:A:227:ILE:O	1:A:228:ASP:OD2	0.47	2.32	7	1
1:A:217:THR:O	1:A:239:ASN:OD1	0.47	2.32	2	2
1:A:242:LEU:CD2	1:A:264:ASP:OD1	0.47	2.63	4	1
1:A:48:ASN:CB	1:A:52:THR:OG1	0.47	2.63	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:LEU:C	1:A:61:LYS:O	0.47	2.54	14	3
1:A:202:LEU:N	1:A:202:LEU:HD12	0.47	2.25	14	2
1:A:3:VAL:CG1	1:A:122:HIS:N	0.46	2.78	6	1
1:A:69:LEU:HD12	1:A:69:LEU:N	0.46	2.26	10	1
1:A:176:ASP:OD1	1:A:176:ASP:O	0.46	2.34	11	2
1:A:184:VAL:HG13	1:A:190:PHE:CD2	0.46	2.45	2	3
1:A:260:SER:OG	1:A:276:GLY:O	0.46	2.33	4	4
1:A:41:PHE:CD2	1:A:60:THR:OG1	0.46	2.63	2	1
1:A:186:ASP:O	1:A:188:THR:HG23	0.46	2.10	5	1
1:A:24:PHE:CD2	1:A:24:PHE:N	0.46	2.82	14	1
1:A:24:PHE:CE1	1:A:262:LEU:HD22	0.46	2.46	7	1
1:A:178:PHE:CD1	1:A:178:PHE:C	0.46	2.85	15	2
1:A:97:LEU:C	1:A:97:LEU:HD13	0.46	2.30	15	1
1:A:227:ILE:HB	1:A:229:PRO:CD	0.46	2.41	18	1
1:A:77:THR:C	1:A:79:ASN:N	0.46	2.69	9	5
1:A:103:PHE:CD1	1:A:110:LYS:NZ	0.46	2.81	5	1
1:A:5:PRO:O	1:A:6:THR:C	0.46	2.54	12	8
1:A:239:ASN:C	1:A:239:ASN:ND2	0.46	2.67	15	1
1:A:210:TRP:CD1	1:A:217:THR:OG1	0.46	2.62	18	1
1:A:173:TYR:CD1	1:A:180:LEU:HD23	0.46	2.46	19	1
1:A:183:ASN:O	1:A:183:ASN:OD1	0.46	2.33	2	1
1:A:262:LEU:HD23	1:A:274:LYS:CD	0.46	2.40	13	1
1:A:239:ASN:ND2	1:A:239:ASN:C	0.46	2.67	2	1
1:A:177:GLU:OE1	1:A:177:GLU:N	0.46	2.49	6	1
1:A:178:PHE:N	1:A:178:PHE:CD1	0.46	2.78	16	2
1:A:178:PHE:CD2	1:A:179:GLN:N	0.46	2.84	14	2
1:A:41:PHE:CE2	1:A:60:THR:CG2	0.46	2.99	16	5
1:A:175:THR:O	1:A:176:ASP:C	0.46	2.54	8	5
1:A:175:THR:OG1	1:A:178:PHE:CG	0.46	2.69	12	1
1:A:77:THR:C	1:A:79:ASN:H	0.46	2.14	1	2
1:A:62:TYR:CE2	1:A:64:TRP:CD1	0.46	3.04	4	3
1:A:145:GLY:O	1:A:146:TYR:CD2	0.46	2.68	18	1
1:A:165:THR:OG1	1:A:166:GLN:N	0.46	2.48	1	3
1:A:166:GLN:NE2	1:A:186:ASP:OD1	0.46	2.49	1	1
1:A:68:GLY:O	1:A:86:THR:O	0.46	2.34	1	8
1:A:178:PHE:C	1:A:178:PHE:CD1	0.46	2.87	19	1
1:A:3:VAL:C	1:A:124:ASN:HD21	0.45	2.14	11	1
1:A:202:LEU:HD12	1:A:202:LEU:N	0.45	2.25	4	1
1:A:113:LYS:NZ	1:A:139:ARG:HH12	0.45	2.10	2	1
1:A:225:TYR:O	1:A:225:TYR:CG	0.45	2.70	5	2
1:A:157:PHE:CD2	1:A:164:VAL:HG22	0.45	2.46	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:238:ASN:OD1	1:A:242:LEU:O	0.45	2.35	13	7
1:A:259:LEU:HD12	1:A:259:LEU:N	0.45	2.26	1	1
1:A:169:PHE:O	1:A:183:ASN:OD1	0.45	2.33	9	2
1:A:41:PHE:CE1	1:A:60:THR:CG2	0.45	2.99	14	5
1:A:7:TYR:CE2	1:A:183:ASN:CB	0.45	3.00	9	1
1:A:175:THR:OG1	1:A:178:PHE:CD2	0.45	2.65	15	3
1:A:93:ARG:O	1:A:119:LYS:O	0.45	2.34	18	1
1:A:6:THR:CG2	1:A:124:ASN:ND2	0.45	2.79	1	1
1:A:143:VAL:HG22	1:A:152:GLY:CA	0.45	2.41	1	1
1:A:168:ASN:OD1	1:A:185:ASN:OD1	0.45	2.35	7	4
1:A:139:ARG:CZ	1:A:156:ASN:ND2	0.45	2.79	20	2
1:A:47:ALA:HA	1:A:53:LYS:O	0.45	2.11	4	12
1:A:139:ARG:HH21	1:A:156:ASN:ND2	0.45	2.09	11	1
1:A:219:PHE:CE2	1:A:239:ASN:CB	0.45	3.00	11	1
1:A:46:SER:OG	1:A:55:THR:O	0.45	2.35	6	3
1:A:250:THR:CG2	1:A:255:ILE:O	0.45	2.64	16	3
1:A:134:ALA:O	1:A:160:ALA:HB3	0.45	2.11	6	1
1:A:46:SER:OG	1:A:55:THR:OG1	0.45	2.35	11	2
1:A:241:SER:OG	1:A:264:ASP:OD2	0.45	2.35	15	1
1:A:231:ALA:C	1:A:232:CYS:SG	0.45	2.95	1	2
1:A:78:ASP:O	1:A:79:ASN:CG	0.45	2.55	7	12
1:A:178:PHE:CD2	1:A:178:PHE:C	0.45	2.90	9	2
1:A:75:TRP:CD1	1:A:75:TRP:C	0.45	2.89	3	2
1:A:227:ILE:CG2	1:A:228:ASP:N	0.45	2.80	14	2
1:A:98:THR:HG22	1:A:98:THR:O	0.45	2.11	13	2
1:A:118:TYR:OH	1:A:120:ARG:NE	0.45	2.50	15	1
1:A:56:GLY:C	1:A:57:SER:OG	0.45	2.55	19	1
1:A:202:LEU:CG	1:A:203:GLU:N	0.44	2.80	7	1
1:A:88:GLU:O	1:A:89:ASP:CB	0.44	2.65	9	1
1:A:175:THR:C	1:A:177:GLU:H	0.44	2.14	18	3
1:A:7:TYR:CZ	1:A:8:ALA:HB2	0.44	2.47	20	1
1:A:49:THR:HG22	1:A:50:GLU:N	0.44	2.26	9	1
1:A:67:TYR:O	1:A:69:LEU:CD1	0.44	2.65	10	1
1:A:5:PRO:N	1:A:119:LYS:NZ	0.44	2.65	18	1
1:A:259:LEU:N	1:A:259:LEU:HD12	0.44	2.27	19	1
1:A:5:PRO:HG2	1:A:143:VAL:HG11	0.44	1.87	1	1
1:A:5:PRO:O	1:A:6:THR:CB	0.44	2.64	1	1
1:A:177:GLU:CD	1:A:197:LYS:O	0.44	2.56	2	1
1:A:178:PHE:CG	1:A:196:GLN:NE2	0.44	2.85	12	1
1:A:225:TYR:CG	1:A:225:TYR:O	0.44	2.71	15	1
1:A:121:GLU:C	1:A:123:ILE:H	0.44	2.15	10	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:TYR:CD1	1:A:170:ALA:CB	0.44	3.01	2	1
1:A:30:ASP:OD2	1:A:42:THR:HG23	0.44	2.11	14	3
1:A:136:PRO:O	1:A:159:THR:OG1	0.44	2.31	5	5
1:A:203:GLU:O	1:A:204:THR:CG2	0.44	2.65	5	3
1:A:153:TYR:CZ	1:A:167:SER:OG	0.44	2.70	9	1
1:A:100:ASP:OD2	1:A:101:SER:N	0.44	2.51	11	2
1:A:102:SER:OG	1:A:111:ASN:ND2	0.44	2.51	11	1
1:A:219:PHE:CE2	1:A:239:ASN:CG	0.44	2.90	18	1
1:A:143:VAL:HA	1:A:151:ALA:O	0.44	2.12	1	1
1:A:195:TYR:CE1	1:A:203:GLU:OE1	0.44	2.71	4	1
1:A:46:SER:CB	1:A:55:THR:O	0.44	2.65	13	3
1:A:202:LEU:HD23	1:A:224:LYS:O	0.44	2.13	7	1
1:A:5:PRO:C	1:A:124:ASN:HD21	0.44	2.14	9	2
1:A:169:PHE:O	1:A:183:ASN:CG	0.44	2.56	9	1
1:A:175:THR:HG1	1:A:178:PHE:N	0.44	2.10	16	2
1:A:225:TYR:C	1:A:225:TYR:CD1	0.44	2.89	5	1
1:A:47:ALA:CB	1:A:53:LYS:O	0.44	2.66	14	7
1:A:6:THR:CG2	1:A:141:ALA:HB3	0.44	2.40	2	2
1:A:6:THR:O	1:A:7:TYR:C	0.44	2.56	1	6
1:A:36:GLU:O	1:A:37:ASN:O	0.44	2.36	6	1
1:A:250:THR:HG22	1:A:250:THR:O	0.44	2.13	9	1
1:A:183:ASN:C	1:A:183:ASN:OD1	0.44	2.55	10	1
1:A:30:ASP:C	1:A:30:ASP:OD1	0.44	2.56	20	2
1:A:74:LYS:HZ1	1:A:76:ASN:ND2	0.44	2.11	20	1
1:A:230:ASP:CG	1:A:250:THR:O	0.44	2.56	5	2
1:A:178:PHE:CD1	1:A:179:GLN:N	0.44	2.85	19	1
1:A:111:ASN:N	1:A:111:ASN:ND2	0.43	2.66	14	1
1:A:7:TYR:CZ	1:A:168:ASN:ND2	0.43	2.86	1	1
1:A:178:PHE:CE2	1:A:196:GLN:NE2	0.43	2.86	5	1
1:A:65:THR:C	1:A:67:TYR:H	0.43	2.16	9	1
1:A:140:GLY:O	1:A:154:GLN:CD	0.43	2.57	16	2
1:A:139:ARG:NH1	1:A:166:GLN:OE1	0.43	2.51	4	1
1:A:175:THR:HG1	1:A:178:PHE:H	0.43	1.54	18	3
1:A:13:SER:OG	1:A:195:TYR:CE1	0.43	2.64	9	1
1:A:145:GLY:HA2	1:A:149:TRP:O	0.43	2.13	14	3
1:A:97:LEU:CD1	1:A:116:THR:OG1	0.43	2.66	20	2
1:A:30:ASP:OD2	1:A:42:THR:CG2	0.43	2.66	16	2
1:A:238:ASN:OD1	1:A:242:LEU:CD1	0.43	2.66	3	1
1:A:87:VAL:CG1	1:A:87:VAL:O	0.43	2.66	3	1
1:A:10:LEU:HD21	1:A:181:HIS:NE2	0.43	2.29	13	1
1:A:5:PRO:O	1:A:6:THR:OG1	0.43	2.36	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:175:THR:CG2	1:A:178:PHE:CE1	0.43	2.97	9	1
1:A:24:PHE:CG	1:A:262:LEU:HD12	0.43	2.49	11	1
1:A:227:ILE:HG23	1:A:231:ALA:CB	0.43	2.43	9	1
1:A:264:ASP:O	1:A:265:GLY:C	0.43	2.57	12	2
1:A:190:PHE:CD2	1:A:210:TRP:CZ2	0.43	3.06	10	1
1:A:98:THR:O	1:A:98:THR:HG22	0.43	2.14	12	1
1:A:202:LEU:HD11	1:A:225:TYR:CE1	0.43	2.49	11	2
1:A:225:TYR:CD2	1:A:227:ILE:HG22	0.43	2.48	13	1
1:A:2:ALA:O	1:A:3:VAL:C	0.43	2.56	1	1
1:A:149:TRP:HD1	1:A:149:TRP:N	0.43	2.06	18	2
1:A:30:ASP:OD1	1:A:42:THR:CG2	0.43	2.66	15	1
1:A:10:LEU:CD2	1:A:181:HIS:CE1	0.43	3.00	16	3
1:A:10:LEU:C	1:A:10:LEU:HD23	0.43	2.33	18	2
1:A:176:ASP:O	1:A:176:ASP:OD1	0.43	2.37	20	1
1:A:238:ASN:C	1:A:238:ASN:OD1	0.43	2.57	1	2
1:A:51:THR:C	1:A:52:THR:OG1	0.43	2.57	2	9
1:A:247:TYR:CE2	1:A:249:GLN:CG	0.43	3.02	5	1
1:A:225:TYR:CD1	1:A:225:TYR:C	0.43	2.92	7	2
1:A:154:GLN:O	1:A:167:SER:OG	0.42	2.31	4	1
1:A:167:SER:C	1:A:168:ASN:ND2	0.42	2.72	11	1
1:A:278:GLY:C	1:A:279:LEU:HD12	0.42	2.34	14	1
1:A:126:GLY:O	1:A:140:GLY:CA	0.42	2.68	1	1
1:A:30:ASP:C	1:A:30:ASP:OD2	0.42	2.56	3	3
1:A:182:THR:O	1:A:183:ASN:OD1	0.42	2.36	4	1
1:A:158:GLU:OE1	1:A:163:ARG:O	0.42	2.36	5	1
1:A:260:SER:OG	1:A:276:GLY:CA	0.42	2.67	20	1
1:A:279:LEU:N	1:A:279:LEU:HD12	0.42	2.29	14	1
1:A:41:PHE:CD1	1:A:60:THR:OG1	0.42	2.64	14	1
1:A:177:GLU:OE2	1:A:197:LYS:O	0.42	2.37	1	1
1:A:71:PHE:CD2	1:A:71:PHE:N	0.42	2.88	11	2
1:A:75:TRP:C	1:A:75:TRP:CD1	0.42	2.90	2	1
1:A:69:LEU:HD22	1:A:87:VAL:HG22	0.42	1.91	4	1
1:A:18:PHE:CD2	1:A:207:ASN:ND2	0.42	2.87	6	1
1:A:2:ALA:HB2	1:A:174:LYS:HZ3	0.42	1.71	9	1
1:A:183:ASN:OD1	1:A:183:ASN:C	0.42	2.57	14	2
1:A:156:ASN:OD1	1:A:166:GLN:OE1	0.42	2.37	5	1
1:A:51:THR:O	1:A:52:THR:OG1	0.42	2.37	12	5
1:A:175:THR:O	1:A:178:PHE:N	0.42	2.52	8	1
1:A:241:SER:O	1:A:265:GLY:CA	0.42	2.68	12	1
1:A:93:ARG:CD	1:A:120:ARG:HH21	0.42	2.27	18	1
1:A:4:PRO:C	1:A:124:ASN:HD22	0.42	2.17	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:238:ASN:OD1	1:A:238:ASN:C	0.42	2.57	2	1
1:A:10:LEU:CD2	1:A:10:LEU:N	0.42	2.83	3	1
1:A:202:LEU:HD11	1:A:225:TYR:CE2	0.42	2.50	4	1
1:A:225:TYR:CE1	1:A:227:ILE:HB	0.42	2.49	5	1
1:A:7:TYR:CE2	1:A:168:ASN:CB	0.42	3.02	8	1
1:A:240:SER:O	1:A:241:SER:OG	0.42	2.35	18	1
1:A:264:ASP:OD2	1:A:264:ASP:C	0.42	2.58	1	2
1:A:102:SER:O	1:A:109:LYS:O	0.42	2.37	2	2
1:A:250:THR:HG22	1:A:256:LYS:NZ	0.42	2.29	3	1
1:A:87:VAL:O	1:A:87:VAL:CG1	0.42	2.67	9	1
1:A:47:ALA:HB1	1:A:53:LYS:O	0.42	2.15	14	1
1:A:28:LYS:NZ	1:A:44:SER:OG	0.42	2.52	20	1
1:A:202:LEU:HD23	1:A:226:GLN:HB3	0.42	1.90	5	1
1:A:128:ASP:C	1:A:128:ASP:OD1	0.42	2.58	8	1
1:A:282:GLN:O	1:A:283:ALA:CB	0.42	2.66	11	1
1:A:175:THR:OG1	1:A:178:PHE:CB	0.42	2.67	12	1
1:A:63:ARG:NH1	1:A:65:THR:HG21	0.42	2.30	16	2
1:A:233:PHE:CE1	1:A:235:ALA:HB2	0.42	2.50	18	1
1:A:122:HIS:CG	1:A:145:GLY:O	0.42	2.73	7	2
1:A:102:SER:O	1:A:103:PHE:CB	0.42	2.67	9	2
1:A:114:ILE:O	1:A:127:CYS:O	0.42	2.37	9	1
1:A:103:PHE:N	1:A:103:PHE:CD2	0.42	2.87	12	1
1:A:196:GLN:HB3	1:A:204:THR:OG1	0.42	2.15	12	1
1:A:102:SER:OG	1:A:103:PHE:CD1	0.41	2.73	12	1
1:A:220:GLY:HA2	1:A:238:ASN:HA	0.41	1.92	16	2
1:A:219:PHE:C	1:A:219:PHE:CD1	0.41	2.94	3	1
1:A:177:GLU:OE1	1:A:178:PHE:CZ	0.41	2.73	4	1
1:A:260:SER:CB	1:A:276:GLY:O	0.41	2.68	12	2
1:A:178:PHE:CE1	1:A:196:GLN:OE1	0.41	2.73	8	1
1:A:37:ASN:O	1:A:37:ASN:OD1	0.41	2.38	11	1
1:A:18:PHE:CB	1:A:207:ASN:HD22	0.41	2.28	12	1
1:A:168:ASN:OD1	1:A:184:VAL:O	0.41	2.38	2	2
1:A:3:VAL:HG13	1:A:122:HIS:H	0.41	1.75	6	1
1:A:202:LEU:HD22	1:A:226:GLN:HB2	0.41	1.92	7	1
1:A:177:GLU:OE2	1:A:178:PHE:CZ	0.41	2.73	20	2
1:A:238:ASN:HD21	1:A:242:LEU:HG	0.41	1.75	14	1
1:A:164:VAL:O	1:A:165:THR:CG2	0.41	2.68	4	4
1:A:132:ASP:OD2	1:A:133:ILE:N	0.41	2.53	7	1
1:A:68:GLY:C	1:A:69:LEU:HD12	0.41	2.36	10	1
1:A:219:PHE:O	1:A:238:ASN:HA	0.41	2.15	16	2
1:A:230:ASP:OD2	1:A:231:ALA:N	0.41	2.54	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:172:GLY:CA	1:A:180:LEU:O	0.41	2.69	16	3
1:A:2:ALA:O	1:A:3:VAL:CG1	0.41	2.69	11	2
1:A:39:LEU:O	1:A:40:GLU:C	0.41	2.59	14	1
1:A:62:TYR:O	1:A:69:LEU:O	0.41	2.37	14	1
1:A:263:LEU:CD1	1:A:263:LEU:N	0.41	2.82	2	1
1:A:228:ASP:CB	1:A:229:PRO:CD	0.41	2.99	20	2
1:A:3:VAL:CA	1:A:124:ASN:OD1	0.41	2.69	4	1
1:A:30:ASP:OD1	1:A:43:SER:O	0.41	2.38	11	1
1:A:225:TYR:CE2	1:A:227:ILE:HG23	0.41	2.51	20	1
1:A:5:PRO:O	1:A:10:LEU:CD1	0.41	2.68	14	1
1:A:39:LEU:O	1:A:40:GLU:O	0.41	2.38	14	1
1:A:238:ASN:HD21	1:A:242:LEU:HD12	0.41	1.75	20	1
1:A:176:ASP:C	1:A:178:PHE:N	0.41	2.74	1	1
1:A:5:PRO:CA	1:A:119:LYS:HZ1	0.41	2.29	8	1
1:A:183:ASN:OD1	1:A:191:GLY:O	0.41	2.37	13	1
1:A:140:GLY:O	1:A:154:GLN:OE1	0.41	2.39	16	2
1:A:56:GLY:O	1:A:57:SER:OG	0.41	2.36	19	1
1:A:271:GLY:O	1:A:273:HIS:ND1	0.41	2.53	1	1
1:A:170:ALA:HB2	1:A:183:ASN:ND2	0.41	2.30	3	1
1:A:144:LEU:N	1:A:144:LEU:HD22	0.41	2.31	10	1
1:A:227:ILE:HG21	1:A:227:ILE:HD13	0.41	1.74	19	1
1:A:190:PHE:CB	1:A:210:TRP:CE2	0.40	3.05	5	1
1:A:168:ASN:ND2	1:A:168:ASN:N	0.40	2.68	8	1
1:A:39:LEU:O	1:A:61:LYS:N	0.40	2.54	12	1
1:A:110:LYS:C	1:A:111:ASN:HD22	0.40	2.19	14	1
1:A:151:ALA:HB1	1:A:170:ALA:O	0.40	2.17	14	1
1:A:95:LEU:CD2	1:A:95:LEU:C	0.40	2.90	2	1
1:A:202:LEU:CD1	1:A:202:LEU:N	0.40	2.84	4	1
1:A:216:ASN:OD1	1:A:216:ASN:O	0.40	2.39	7	1
1:A:157:PHE:CE2	1:A:164:VAL:HG23	0.40	2.50	9	1
1:A:271:GLY:O	1:A:272:GLY:C	0.40	2.59	14	1
1:A:65:THR:O	1:A:66:GLU:C	0.40	2.60	14	1
1:A:51:THR:OG1	1:A:53:LYS:CG	0.40	2.70	1	1
1:A:102:SER:O	1:A:103:PHE:CG	0.40	2.75	9	1
1:A:194:ILE:O	1:A:205:ALA:HB1	0.40	2.17	16	2
1:A:242:LEU:HD11	1:A:264:ASP:CG	0.40	2.37	16	2
1:A:3:VAL:C	1:A:124:ASN:OD1	0.40	2.60	4	1
1:A:237:VAL:O	1:A:237:VAL:HG22	0.40	2.16	9	1
1:A:180:LEU:HD23	1:A:180:LEU:C	0.40	2.36	15	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	253/285 (89%)	223±3 (88±1%)	20±3 (8±1%)	10±2 (4±1%)	6	33
All	All	5060/5700 (89%)	4458 (88%)	401 (8%)	201 (4%)	6	33

All 33 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	121	GLU	19
1	A	122	HIS	19
1	A	79	ASN	18
1	A	120	ARG	14
1	A	24	PHE	13
1	A	241	SER	11
1	A	49	THR	9
1	A	176	ASP	9
1	A	109	LYS	9
1	A	94	GLY	8
1	A	65	THR	7
1	A	147	GLU	7
1	A	66	GLU	7
1	A	265	GLY	6
1	A	37	ASN	5
1	A	228	ASP	4
1	A	202	LEU	4
1	A	229	PRO	4
1	A	93	ARG	3
1	A	250	THR	3
1	A	177	GLU	3
1	A	283	ALA	3
1	A	230	ASP	2
1	A	38	GLY	2
1	A	64	TRP	2
1	A	40	GLU	2
1	A	63	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	51	THR	1
1	A	7	TYR	1
1	A	89	ASP	1
1	A	5	PRO	1
1	A	6	THR	1
1	A	36	GLU	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	207/232 (89%)	195±2 (94±1%)	12±2 (6±1%)	29	75
All	All	4140/4640 (89%)	3901 (94%)	239 (6%)	29	75

All 51 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	7	TYR	18
1	A	228	ASP	18
1	A	102	SER	17
1	A	157	PHE	16
1	A	178	PHE	16
1	A	227	ILE	14
1	A	52	THR	11
1	A	124	ASN	11
1	A	101	SER	10
1	A	210	TRP	10
1	A	3	VAL	9
1	A	241	SER	8
1	A	51	THR	5
1	A	175	THR	5
1	A	262	LEU	4
1	A	202	LEU	4
1	A	156	ASN	4
1	A	238	ASN	4
1	A	57	SER	4

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Mol	Chain	Res	Type	Models (Total)
1	A	230	ASP	3
1	A	237	VAL	3
1	A	65	THR	3
1	A	193	SER	3
1	A	154	GLN	3
1	A	232	CYS	2
1	A	168	ASN	2
1	A	40	GLU	2
1	A	196	GLN	2
1	A	49	THR	2
1	A	150	LEU	2
1	A	208	LEU	2
1	A	97	LEU	2
1	A	239	ASN	2
1	A	280	GLU	1
1	A	233	PHE	1
1	A	259	LEU	1
1	A	128	ASP	1
1	A	146	TYR	1
1	A	242	LEU	1
1	A	183	ASN	1
1	A	84	GLU	1
1	A	71	PHE	1
1	A	180	LEU	1
1	A	39	LEU	1
1	A	207	ASN	1
1	A	87	VAL	1
1	A	86	THR	1
1	A	190	PHE	1
1	A	279	LEU	1
1	A	59	GLU	1
1	A	211	THR	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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: 5jdp_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping

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

Total number of shifts	971
Number of shifts mapped to atoms	0
Number of unparsed shifts	971
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

- Entity instance (chain) must be specified. All 971 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	6	THR	H	7.426	0.005	1
2	?	6	THR	N	106.255	0.023	1
3	?	7	TYR	H	7.660	0.005	1
4	?	7	TYR	N	122.565	0.108	1
5	?	166	GLN	H	7.442	0.008	1
6	?	166	GLN	N	120.974	0.058	1
7	?	244	GLY	H	9.294	0.012	1
8	?	244	GLY	N	114.566	0.075	1
9	?	43	SER	H	9.211	0.005	1
10	?	43	SER	N	120.790	0.087	1
11	?	123	ILE	H	7.926	0.009	1
12	?	123	ILE	N	117.980	0.088	1
13	?	134	ALA	H	8.459	0.004	1
14	?	134	ALA	N	123.455	0.029	1
15	?	210	TRP	H	9.001	0.009	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
16	?	210	TRP	N	121.358	0.03	1
17	?	91	LEU	H	8.273	0.013	1
18	?	91	LEU	N	117.676	0.033	1
19	?	187	GLY	H	8.644	0.007	1
20	?	187	GLY	N	105.249	0.067	1
21	?	120	ARG	H	8.715	0.007	1
22	?	120	ARG	N	117.760	0.107	1
23	?	127	CYS	H	8.538	0.01	1
24	?	127	CYS	N	121.238	0.056	1
25	?	142	LEU	H	9.222	0.008	1
26	?	142	LEU	N	123.770	0.054	1
27	?	81	LEU	H	8.623	0.009	1
28	?	81	LEU	N	128.129	0.099	1
29	?	68	GLY	H	7.563	0.006	1
30	?	68	GLY	N	105.520	0.054	1
31	?	150	LEU	H	8.964	0.007	1
32	?	150	LEU	N	123.407	0.07	1
33	?	267	ASN	H	7.417	0.006	1
34	?	267	ASN	N	117.429	0.052	1
35	?	139	ARG	H	9.052	0.009	1
36	?	139	ARG	N	128.477	0.063	1
37	?	220	GLY	H	8.575	0.008	1
38	?	220	GLY	N	107.697	0.072	1
39	?	103	PHE	H	9.057	0.005	1
40	?	103	PHE	N	121.168	0.049	1
41	?	270	ALA	H	7.494	0.007	1
42	?	270	ALA	N	120.589	0.044	1
43	?	83	THR	H	8.808	0.007	1
44	?	83	THR	N	114.152	0.025	1
45	?	125	LEU	H	9.480	0.006	1
46	?	125	LEU	N	128.898	0.066	1
47	?	277	LEU	H	8.231	0.005	1
48	?	277	LEU	N	120.912	0.046	1
49	?	89	ASP	H	8.738	0.008	1
50	?	89	ASP	N	118.050	0.073	1
51	?	225	TYR	H	9.859	0.005	1
52	?	225	TYR	N	128.980	0.101	1
53	?	64	TRP	H	9.132	0.006	1
54	?	64	TRP	N	128.001	0.098	1
55	?	224	LYS	H	8.758	0.01	1
56	?	224	LYS	N	122.474	0.023	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
57	?	135	GLY	H	7.644	0.003	1
58	?	135	GLY	N	106.332	0.027	1
59	?	266	LYS	H	8.133	0.005	1
60	?	266	LYS	N	117.235	0.051	1
61	?	15	ARG	H	7.305	0.006	1
62	?	15	ARG	N	117.280	0.062	1
63	?	271	GLY	H	7.667	0.006	1
64	?	271	GLY	N	106.689	0.111	1
65	?	155	MET	H	8.759	0.007	1
66	?	155	MET	N	121.345	0.092	1
67	?	181	HIS	H	9.147	0.006	1
68	?	181	HIS	N	128.679	0.044	1
69	?	145	GLY	H	8.145	0.004	1
70	?	145	GLY	N	105.144	0.033	1
71	?	88	GLU	H	9.099	0.012	1
72	?	88	GLU	N	128.396	0.047	1
73	?	208	LEU	H	8.700	0.006	1
74	?	208	LEU	N	121.396	0.033	1
75	?	59	GLU	H	9.017	0.006	1
76	?	59	GLU	N	123.531	0.055	1
77	?	192	GLY	H	8.628	0.011	1
78	?	192	GLY	N	105.554	0.042	1
79	?	117	GLY	H	9.178	0.007	1
80	?	117	GLY	N	113.659	0.054	1
81	?	27	ILE	H	8.696	0.004	1
82	?	27	ILE	N	120.947	0.025	1
83	?	254	GLY	H	8.549	0.005	1
84	?	254	GLY	N	110.659	0.096	1
85	?	118	TYR	H	9.107	0.007	1
86	?	118	TYR	N	123.138	0.114	1
87	?	246	GLY	H	9.187	0.008	1
88	?	246	GLY	N	110.634	0.074	1
89	?	42	THR	H	8.847	0.008	1
90	?	42	THR	N	120.659	0.062	1
91	?	76	ASN	H	7.624	0.011	1
92	?	76	ASN	N	123.089	0.025	1
93	?	193	SER	H	9.754	0.008	1
94	?	193	SER	N	114.615	0.05	1
95	?	57	SER	H	9.086	0.01	1
96	?	57	SER	N	113.059	0.042	1
97	?	216	ASN	H	8.370	0.006	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
98	?	216	ASN	N	120.500	0.15	1
99	?	162	SER	H	7.482	0.008	1
100	?	162	SER	N	114.724	0.076	1
101	?	160	ALA	H	9.124	0.009	1
102	?	160	ALA	N	124.989	0.089	1
103	?	261	ALA	H	9.549	0.009	1
104	?	261	ALA	N	120.637	0.07	1
105	?	230	ASP	H	8.499	0.008	1
106	?	230	ASP	N	114.288	0.022	1
107	?	44	SER	H	8.608	0.008	1
108	?	44	SER	N	120.396	0.066	1
109	?	262	LEU	H	8.735	0.007	1
110	?	262	LEU	N	124.795	0.064	1
111	?	199	ASN	H	8.172	0.013	1
112	?	199	ASN	N	113.551	0.108	1
113	?	40	GLU	H	9.003	0.005	1
114	?	40	GLU	N	124.641	0.064	1
115	?	172	GLY	H	9.426	0.005	1
116	?	172	GLY	N	112.952	0.031	1
117	?	217	THR	H	8.370	0.004	1
118	?	217	THR	N	119.348	0.041	1
119	?	119	LYS	H	7.544	0.014	1
120	?	119	LYS	N	124.832	0.064	1
121	?	279	LEU	H	8.691	0.005	1
122	?	279	LEU	N	124.706	0.06	1
123	?	80	THR	H	7.265	0.01	1
124	?	80	THR	N	112.891	0.085	1
125	?	111	ASN	H	8.562	0.008	1
126	?	111	ASN	N	119.611	0.039	1
127	?	204	THR	H	8.399	0.01	1
128	?	204	THR	N	112.190	0.07	1
129	?	264	ASP	H	9.901	0.013	1
130	?	264	ASP	N	124.571	0.094	1
131	?	82	GLY	H	9.375	0.006	1
132	?	82	GLY	N	112.369	0.075	1
133	?	143	VAL	H	9.018	0.008	1
134	?	143	VAL	N	125.151	0.024	1
135	?	32	LYS	H	8.655	0.011	1
136	?	32	LYS	N	124.807	0.024	1
137	?	265	GLY	H	8.453	0.005	1
138	?	265	GLY	N	112.333	0.055	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
139	?	113	LYS	H	9.046	0.004	1
140	?	113	LYS	N	119.785	0.094	1
141	?	178	PHE	H	7.510	0.006	1
142	?	178	PHE	N	119.852	0.027	1
143	?	156	ASN	H	7.985	0.007	1
144	?	156	ASN	N	119.611	0.107	1
145	?	124	ASN	H	8.968	0.004	1
146	?	124	ASN	N	125.387	0.085	1
147	?	234	SER	H	9.322	0.015	1
148	?	234	SER	N	124.625	0.103	1
149	?	175	THR	H	8.581	0.006	1
150	?	175	THR	N	117.777	0.041	1
151	?	241	SER	H	8.148	0.005	1
152	?	241	SER	N	109.462	0.046	1
153	?	10	LEU	H	7.356	0.003	1
154	?	10	LEU	N	125.355	0.046	1
155	?	223	ALA	H	9.205	0.01	1
156	?	223	ALA	N	119.347	0.061	1
157	?	214	ASN	H	7.960	0.005	1
158	?	214	ASN	N	119.151	0.0	1
159	?	86	THR	H	8.992	0.007	1
160	?	86	THR	N	123.814	0.024	1
161	?	274	LYS	H	8.874	0.007	1
162	?	274	LYS	N	119.348	0.013	1
163	?	163	ARG	H	6.841	0.007	1
164	?	163	ARG	N	115.106	0.051	1
165	?	94	GLY	H	9.431	0.005	1
166	?	94	GLY	N	115.364	0.07	1
167	?	278	GLY	H	9.585	0.009	1
168	?	278	GLY	N	115.873	0.077	1
169	?	60	THR	H	9.065	0.004	1
170	?	60	THR	N	120.015	0.046	1
171	?	84	GLU	H	8.883	0.005	1
172	?	84	GLU	N	124.625	0.044	1
173	?	167	SER	H	8.323	0.008	1
174	?	167	SER	N	118.931	0.044	1
175	?	260	SER	H	8.819	0.009	1
176	?	260	SER	N	115.286	0.068	1
177	?	69	LEU	H	7.244	0.005	1
178	?	69	LEU	N	120.101	0.048	1
179	?	194	ILE	H	8.785	0.006	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
180	?	194	ILE	N	119.009	0.023	1
181	?	9	ASP	H	7.225	0.006	1
182	?	9	ASP	N	115.199	0.064	1
183	?	8	ALA	H	8.412	0.006	1
184	?	8	ALA	N	119.083	0.033	1
185	?	79	ASN	H	8.507	0.005	1
186	?	79	ASN	N	115.074	0.067	1
187	?	219	PHE	H	8.039	0.006	1
188	?	219	PHE	N	119.015	0.069	1
189	?	165	THR	H	8.633	0.004	1
190	?	165	THR	N	118.921	0.022	1
191	?	170	ALA	H	8.826	0.007	1
192	?	170	ALA	N	122.652	0.064	1
193	?	62	TYR	H	9.255	0.007	1
194	?	62	TYR	N	124.077	0.048	1
195	?	236	LYS	H	9.042	0.008	1
196	?	236	LYS	N	114.784	0.092	1
197	?	55	THR	H	8.781	0.005	1
198	?	55	THR	N	118.726	0.037	1
199	?	100	ASP	H	8.680	0.007	1
200	?	100	ASP	N	128.944	0.041	1
201	?	101	SER	H	8.629	0.004	1
202	?	101	SER	N	118.554	0.093	1
203	?	87	VAL	H	9.364	0.004	1
204	?	87	VAL	N	124.751	0.071	1
205	?	195	TYR	H	8.778	0.008	1
206	?	195	TYR	N	127.363	0.085	1
207	?	245	LEU	H	9.385	0.008	1
208	?	245	LEU	N	122.230	0.051	1
209	?	190	PHE	H	8.890	0.012	1
210	?	190	PHE	N	125.704	0.059	1
211	?	275	LEU	H	8.657	0.005	1
212	?	275	LEU	N	121.473	0.019	1
213	?	153	TYR	H	9.211	0.008	1
214	?	153	TYR	N	122.097	0.035	1
215	?	196	GLN	H	8.271	0.01	1
216	?	196	GLN	N	125.550	0.052	1
217	?	185	ASN	H	9.327	0.008	1
218	?	185	ASN	N	129.347	0.052	1
219	?	133	ILE	H	8.446	0.007	1
220	?	133	ILE	N	123.992	0.004	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
221	?	74	LYS	H	9.109	0.006	1
222	?	74	LYS	N	125.784	0.047	1
223	?	285	SER	H	7.845	0.006	1
224	?	285	SER	N	125.650	0.038	1
225	?	280	GLU	H	8.826	0.005	1
226	?	280	GLU	N	125.913	0.049	1
227	?	268	VAL	H	8.514	0.007	1
228	?	268	VAL	N	122.022	0.041	1
229	?	20	LYS	H	7.849	0.006	1
230	?	20	LYS	N	122.023	0.129	1
231	?	157	PHE	H	9.568	0.008	1
232	?	157	PHE	N	127.529	0.06	1
233	?	144	LEU	H	9.351	0.003	1
234	?	144	LEU	N	126.149	0.028	1
235	?	218	ARG	H	9.034	0.005	1
236	?	218	ARG	N	125.653	0.017	1
237	?	281	PHE	H	9.056	0.005	1
238	?	281	PHE	N	126.125	0.03	1
239	?	58	LEU	H	9.048	0.009	1
240	?	58	LEU	N	121.948	0.125	1
241	?	211	THR	H	8.512	0.008	1
242	?	211	THR	N	120.524	0.075	1
243	?	202	LEU	H	7.522	0.005	1
244	?	202	LEU	N	122.055	0.04	1
245	?	257	LEU	H	8.809	0.006	1
246	?	257	LEU	N	127.739	0.103	1
247	?	203	GLU	H	8.842	0.007	1
248	?	203	GLU	N	125.538	0.038	1
249	?	54	VAL	H	8.595	0.007	1
250	?	54	VAL	N	125.749	0.037	1
251	?	112	ALA	H	8.546	0.006	1
252	?	112	ALA	N	124.233	0.017	1
253	?	73	VAL	H	8.985	0.006	1
254	?	73	VAL	N	125.621	0.064	1
255	?	147	GLU	H	9.214	0.004	1
256	?	147	GLU	N	125.645	0.077	1
257	?	180	LEU	H	9.353	0.007	1
258	?	180	LEU	N	127.736	0.046	1
259	?	154	GLN	H	8.217	0.007	1
260	?	154	GLN	N	127.897	0.07	1
261	?	233	PHE	H	9.235	0.004	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
262	?	233	PHE	N	127.738	0.1	1
263	?	226	GLN	H	9.008	0.006	1
264	?	226	GLN	N	131.568	0.072	1
265	?	158	GLU	H	8.089	0.007	1
266	?	158	GLU	N	127.789	0.092	1
267	?	164	VAL	H	8.800	0.008	1
268	?	164	VAL	N	124.310	0.05	1
269	?	63	ARG	H	7.724	0.014	1
270	?	63	ARG	N	127.667	0.127	1
271	?	151	ALA	H	8.872	0.004	1
272	?	151	ALA	N	121.639	0.061	1
273	?	140	GLY	H	8.754	0.007	1
274	?	140	GLY	N	113.394	0.122	1
275	?	149	TRP	H	8.112	0.008	1
276	?	149	TRP	N	121.552	0.054	1
277	?	239	ASN	H	8.463	0.006	1
278	?	239	ASN	N	113.461	0.043	1
279	?	255	ILE	H	8.235	0.006	1
280	?	255	ILE	N	121.494	0.068	1
281	?	240	SER	H	7.807	0.01	1
282	?	240	SER	N	117.033	0.052	1
283	?	191	GLY	H	8.550	0.009	1
284	?	191	GLY	N	110.367	0.065	1
285	?	126	GLY	H	9.473	0.005	1
286	?	126	GLY	N	113.480	0.052	1
287	?	78	ASP	H	7.652	0.006	1
288	?	78	ASP	N	121.076	0.044	1
289	?	26	LEU	H	7.480	0.004	1
290	?	26	LEU	N	118.495	0.061	1
291	?	228	ASP	H	8.429	0.008	1
292	?	228	ASP	N	118.356	0.072	1
293	?	242	LEU	H	7.312	0.009	1
294	?	242	LEU	N	118.495	0.052	1
295	?	35	SER	H	8.791	0.008	1
296	?	35	SER	N	120.131	0.047	1
297	?	205	ALA	H	9.040	0.009	1
298	?	205	ALA	N	122.546	0.085	1
299	?	72	THR	H	9.019	0.006	1
300	?	72	THR	N	120.667	0.04	1
301	?	104	SER	H	7.969	0.005	1
302	?	104	SER	N	120.209	0.027	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
303	?	38	GLY	H	7.841	0.008	1
304	?	38	GLY	N	106.377	0.077	1
305	?	12	LYS	H	7.287	0.006	1
306	?	12	LYS	N	122.430	0.029	1
307	?	110	LYS	H	8.417	0.007	1
308	?	110	LYS	N	123.802	0.041	1
309	?	179	GLN	H	8.701	0.009	1
310	?	179	GLN	N	122.679	0.036	1
311	?	34	LYS	H	8.121	0.014	1
312	?	34	LYS	N	123.889	0.013	1
313	?	67	TYR	H	6.472	0.005	1
314	?	67	TYR	N	113.985	0.081	1
315	?	138	ILE	H	9.109	0.007	1
316	?	138	ILE	N	122.709	0.064	1
317	?	48	ASN	H	8.292	0.006	1
318	?	48	ASN	N	122.218	0.056	1
319	?	207	ASN	H	8.882	0.005	1
320	?	207	ASN	N	122.604	0.052	1
321	?	232	CYS	H	8.465	0.014	1
322	?	232	CYS	N	119.129	0.029	1
323	?	146	TYR	H	8.604	0.01	1
324	?	146	TYR	N	122.413	0.057	1
325	?	184	VAL	H	8.931	0.006	1
326	?	184	VAL	N	118.359	0.058	1
327	?	188	THR	H	7.636	0.009	1
328	?	188	THR	N	109.061	0.054	1
329	?	235	ALA	H	8.031	0.006	1
330	?	235	ALA	N	122.724	0.076	1
331	?	99	PHE	H	9.428	0.008	1
332	?	99	PHE	N	126.829	0.051	1
333	?	39	LEU	H	7.828	0.005	1
334	?	39	LEU	N	122.655	0.059	1
335	?	169	PHE	H	8.621	0.007	1
336	?	169	PHE	N	118.343	0.124	1
337	?	24	PHE	H	7.081	0.009	1
338	?	24	PHE	N	120.114	0.039	1
339	?	95	LEU	H	7.879	0.008	1
340	?	95	LEU	N	122.721	0.043	1
341	?	137	SER	H	8.842	0.006	1
342	?	137	SER	N	118.519	0.073	1
343	?	248	THR	H	8.374	0.01	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
344	?	248	THR	N	124.406	0.039	1
345	?	56	GLY	H	8.307	0.007	1
346	?	56	GLY	N	109.087	0.099	1
347	?	258	THR	H	9.608	0.01	1
348	?	258	THR	N	122.864	0.033	1
349	?	64	TRP	HE1	10.483	0.007	1
350	?	64	TRP	NE1	129.515	0.043	1
351	?	227	ILE	H	7.814	0.008	1
352	?	227	ILE	N	129.908	0.03	1
353	?	148	GLY	H	8.018	0.012	1
354	?	148	GLY	N	107.994	0.084	1
355	?	116	THR	H	8.663	0.01	1
356	?	116	THR	N	117.028	0.072	1
357	?	132	ASP	H	7.353	0.005	1
358	?	132	ASP	N	122.970	0.047	1
359	?	90	GLN	H	7.883	0.007	1
360	?	90	GLN	N	117.023	0.093	1
361	?	25	GLY	H	8.139	0.013	1
362	?	25	GLY	N	110.124	0.149	1
363	?	159	THR	H	7.649	0.006	1
364	?	159	THR	N	116.947	0.037	1
365	?	122	HIS	H	7.880	0.01	1
366	?	122	HIS	N	111.531	0.047	1
367	?	189	GLU	H	7.642	0.006	1
368	?	189	GLU	N	122.909	0.061	1
369	?	149	TRP	HE1	10.610	0.008	1
370	?	149	TRP	NE1	130.026	0.148	1
371	?	197	LYS	H	8.895	0.006	1
372	?	197	LYS	N	130.397	0.147	1
373	?	238	ASN	H	7.574	0.007	1
374	?	238	ASN	N	122.432	0.102	1
375	?	272	GLY	H	8.537	0.005	1
376	?	272	GLY	N	109.182	0.091	1
377	?	152	GLY	H	9.629	0.006	1
378	?	152	GLY	N	107.694	0.047	1
379	?	276	GLY	H	9.095	0.007	1
380	?	276	GLY	N	111.036	0.076	1
381	?	14	ALA	H	8.301	0.007	1
382	?	14	ALA	N	121.916	0.145	1
383	?	108	GLY	H	8.199	0.006	1
384	?	108	GLY	N	111.631	0.031	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
385	?	77	THR	H	8.067	0.009	1
386	?	77	THR	N	108.066	0.084	1
387	?	206	VAL	H	8.955	0.003	1
388	?	206	VAL	N	116.877	0.055	1
389	?	171	VAL	H	8.234	0.004	1
390	?	171	VAL	N	116.754	0.055	1
391	?	213	GLY	H	8.391	0.005	1
392	?	213	GLY	N	110.033	0.042	1
393	?	129	MET	H	9.420	0.01	1
394	?	129	MET	N	122.886	0.071	1
395	?	75	TRP	HE1	10.664	0.005	1
396	?	75	TRP	NE1	130.109	?	1
397	?	259	LEU	H	9.239	0.009	1
398	?	259	LEU	N	129.328	0.092	1
399	?	30	ASP	H	8.499	0.012	1
400	?	30	ASP	N	123.022	0.038	1
401	?	198	VAL	H	8.595	0.01	1
402	?	198	VAL	N	130.967	0.099	1
403	?	269	ASN	H	8.316	0.006	1
404	?	269	ASN	N	116.907	0.079	1
405	?	131	PHE	H	8.542	0.007	1
406	?	131	PHE	N	123.030	0.03	1
407	?	92	ALA	H	7.507	0.01	1
408	?	92	ALA	N	116.547	0.043	1
409	?	183	ASN	H	8.864	0.004	1
410	?	183	ASN	N	116.576	0.041	1
411	?	33	THR	H	9.046	0.006	1
412	?	33	THR	N	115.815	0.085	1
413	?	210	TRP	HE1	10.132	0.004	1
414	?	210	TRP	NE1	131.635	0.053	1
415	?	96	LYS	H	9.628	0.011	1
416	?	96	LYS	N	132.090	0.043	1
417	?	231	ALA	H	7.671	0.013	1
418	?	231	ALA	N	124.121	0.059	1
419	?	70	THR	H	9.063	0.004	1
420	?	70	THR	N	120.315	0.062	1
421	?	114	ILE	H	8.797	0.005	1
422	?	114	ILE	N	120.605	0.044	1
423	?	263	LEU	H	9.506	0.007	1
424	?	263	LEU	N	126.164	0.059	1
425	?	168	ASN	H	9.126	0.006	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
426	?	168	ASN	N	127.257	0.135	1
427	?	141	ALA	H	8.957	0.01	1
428	?	141	ALA	N	123.981	0.061	1
429	?	173	TYR	H	8.592	0.007	1
430	?	173	TYR	N	119.398	0.037	1
431	?	31	LEU	H	9.092	0.004	1
432	?	31	LEU	N	123.852	0.058	1
433	?	71	PHE	H	9.236	0.004	1
434	?	71	PHE	N	127.012	0.053	1
435	?	53	LYS	H	7.535	0.004	1
436	?	53	LYS	N	120.442	0.049	1
437	?	61	LYS	H	8.844	0.008	1
438	?	61	LYS	N	126.824	0.02	1
439	?	222	ALA	H	8.872	0.007	1
440	?	222	ALA	N	126.237	0.034	1
441	?	209	ALA	H	9.186	0.005	1
442	?	209	ALA	N	126.225	0.104	1
443	?	283	ALA	H	8.341	0.009	1
444	?	283	ALA	N	126.465	0.028	1
445	?	85	ILE	H	9.105	0.006	1
446	?	85	ILE	N	126.404	0.076	1
447	?	97	LEU	H	8.745	0.004	1
448	?	97	LEU	N	126.998	0.035	1
449	?	41	PHE	H	8.712	0.008	1
450	?	41	PHE	N	123.987	0.089	1
451	?	29	LEU	H	8.726	0.007	1
452	?	29	LEU	N	124.242	0.11	1
453	?	243	ILE	H	9.055	0.009	1
454	?	243	ILE	N	126.653	0.13	1
455	?	115	LYS	H	9.268	0.01	1
456	?	115	LYS	N	126.664	0.032	1
457	?	130	ASP	H	8.548	0.006	1
458	?	130	ASP	N	124.928	0.071	1
459	?	174	LYS	H	8.804	0.005	1
460	?	174	LYS	N	129.445	0.078	1
461	?	93	ARG	H	8.771	0.01	1
462	?	93	ARG	N	123.933	0.059	1
463	?	121	GLU	H	9.066	0.015	1
464	?	121	GLU	N	120.788	0.078	1
465	?	22	TYR	H	6.609	0.004	1
466	?	22	TYR	N	113.699	0.042	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
467	?	273	HIS	H	7.220	0.008	1
468	?	273	HIS	N	120.751	0.059	1
469	?	212	ALA	H	8.663	0.007	1
470	?	212	ALA	N	127.059	0.068	1
471	?	98	THR	H	9.166	0.008	1
472	?	98	THR	N	120.267	0.056	1
473	?	109	LYS	H	7.512	0.005	1
474	?	109	LYS	N	120.752	0.035	1
475	?	128	ASP	H	9.372	0.008	1
476	?	128	ASP	N	129.857	0.094	1
477	?	47	ALA	H	9.188	0.007	1
478	?	47	ALA	N	123.943	0.021	1
479	?	16	ASP	H	8.534	0.013	1
480	?	16	ASP	N	118.516	0.0	1
481	?	17	VAL	H	7.483	0.01	1
482	?	17	VAL	N	120.232	0.079	1
483	?	28	LYS	H	8.752	0.007	1
484	?	28	LYS	N	126.875	0.06	1
485	?	45	GLY	H	9.116	0.01	1
486	?	45	GLY	N	111.231	0.041	1
487	?	46	SER	H	9.054	0.005	1
488	?	46	SER	N	116.020	0.02	1
489	?	75	TRP	H	9.105	0.003	1
490	?	75	TRP	N	124.127	0.062	1
491	?	102	SER	H	8.628	0.003	1
492	?	102	SER	N	118.576	0.045	1
493	?	186	ASP	H	9.020	0.008	1
494	?	186	ASP	N	125.172	0.035	1
495	?	237	VAL	H	8.955	0.007	1
496	?	237	VAL	N	116.867	0.03	1
497	?	221	ILE	H	8.802	0.011	1
498	?	221	ILE	N	118.706	0.057	1
499	?	247	TYR	H	9.106	0.004	1
500	?	247	TYR	N	125.497	0.089	1
501	?	249	GLN	H	9.057	0.007	1
502	?	249	GLN	N	125.901	0.042	1
503	?	256	LYS	H	8.680	0.009	1
504	?	256	LYS	N	126.990	0.033	1
505	?	149	TRP	HZ2	7.448	?	1
506	?	6	THR	CA	60.136	0.005	1
507	?	5	PRO	CA	61.107	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
508	?	7	TYR	CA	61.931	0.032	1
509	?	8	ALA	CA	53.566	0.002	1
510	?	9	ASP	CA	53.579	0.01	1
511	?	10	LEU	CA	55.927	?	1
512	?	11	GLY	CA	44.583	?	1
513	?	12	LYS	CA	59.506	?	1
514	?	14	ALA	CA	54.863	0.005	1
515	?	13	SER	CA	62.699	?	1
516	?	15	ARG	CA	59.650	?	1
517	?	17	VAL	CA	66.329	?	1
518	?	16	ASP	CA	56.895	?	1
519	?	20	LYS	CA	60.495	?	1
520	?	21	GLY	CA	44.136	?	1
521	?	22	TYR	CA	55.794	?	1
522	?	24	PHE	CA	56.115	0.03	1
523	?	25	GLY	CA	45.272	0.019	1
524	?	26	LEU	CA	53.058	0.001	1
525	?	27	ILE	CA	59.774	0.001	1
526	?	28	LYS	CA	54.865	?	1
527	?	29	LEU	CA	53.260	0.012	1
528	?	30	ASP	CA	53.432	0.017	1
529	?	31	LEU	CA	53.646	0.001	1
530	?	32	LYS	CA	54.973	0.029	1
531	?	33	THR	CA	60.081	0.058	1
532	?	34	LYS	CA	55.128	0.01	1
533	?	35	SER	CA	57.035	?	1
534	?	37	ASN	CA	52.741	?	1
535	?	38	GLY	CA	45.009	0.024	1
536	?	39	LEU	CA	55.006	0.0	1
537	?	40	GLU	CA	54.871	0.001	1
538	?	41	PHE	CA	56.440	0.039	1
539	?	42	THR	CA	60.853	0.014	1
540	?	43	SER	CA	56.459	0.003	1
541	?	44	SER	CA	56.451	0.005	1
542	?	45	GLY	CA	44.841	0.005	1
543	?	46	SER	CA	56.669	0.015	1
544	?	47	ALA	CA	49.292	0.028	1
545	?	48	ASN	CA	52.538	0.001	1
546	?	53	LYS	CA	56.389	0.002	1
547	?	54	VAL	CA	59.848	0.001	1
548	?	55	THR	CA	59.701	0.022	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
549	?	56	GLY	CA	45.318	0.008	1
550	?	57	SER	CA	57.217	0.03	1
551	?	58	LEU	CA	53.834	0.03	1
552	?	59	GLU	CA	54.664	0.004	1
553	?	60	THR	CA	60.626	0.029	1
554	?	61	LYS	CA	54.060	0.005	1
555	?	62	TYR	CA	56.972	0.002	1
556	?	63	ARG	CA	54.246	0.007	1
557	?	64	TRP	CA	53.290	?	1
558	?	66	GLU	CA	59.038	?	1
559	?	67	TYR	CA	55.890	0.038	1
560	?	68	GLY	CA	46.658	0.007	1
561	?	69	LEU	CA	53.477	0.002	1
562	?	70	THR	CA	62.096	0.047	1
563	?	71	PHE	CA	55.443	0.022	1
564	?	72	THR	CA	61.242	0.013	1
565	?	73	VAL	CA	60.517	0.023	1
566	?	74	LYS	CA	54.348	0.027	1
567	?	75	TRP	CA	55.401	0.03	1
568	?	76	ASN	CA	51.304	0.024	1
569	?	77	THR	CA	63.637	0.001	1
570	?	78	ASP	CA	53.986	0.01	1
571	?	79	ASN	CA	53.894	0.012	1
572	?	80	THR	CA	62.559	0.041	1
573	?	81	LEU	CA	52.953	0.0	1
574	?	82	GLY	CA	44.277	0.007	1
575	?	83	THR	CA	59.472	0.025	1
576	?	84	GLU	CA	54.350	0.001	1
577	?	85	ILE	CA	59.992	0.001	1
578	?	86	THR	CA	60.642	0.005	1
579	?	87	VAL	CA	59.571	0.0	1
580	?	88	GLU	CA	55.057	0.026	1
581	?	89	ASP	CA	56.943	0.061	1
582	?	90	GLN	CA	55.103	0.018	1
583	?	91	LEU	CA	58.272	0.046	1
584	?	92	ALA	CA	51.069	0.016	1
585	?	93	ARG	CA	57.547	0.028	1
586	?	94	GLY	CA	45.009	0.003	1
587	?	95	LEU	CA	53.748	0.034	1
588	?	96	LYS	CA	55.126	0.006	1
589	?	97	LEU	CA	53.460	0.033	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
590	?	98	THR	CA	61.129	0.017	1
591	?	99	PHE	CA	55.836	0.018	1
592	?	100	ASP	CA	52.229	0.018	1
593	?	102	SER	CA	56.982	0.045	1
594	?	103	PHE	CA	55.764	0.02	1
595	?	104	SER	CA	53.253	?	1
596	?	108	GLY	CA	45.217	0.005	1
597	?	109	LYS	CA	56.567	0.005	1
598	?	110	LYS	CA	54.675	0.005	1
599	?	111	ASN	CA	52.621	0.003	1
600	?	112	ALA	CA	51.471	0.003	1
601	?	113	LYS	CA	54.560	0.01	1
602	?	114	ILE	CA	59.265	0.007	1
603	?	115	LYS	CA	54.645	0.016	1
604	?	116	THR	CA	60.092	0.018	1
605	?	117	GLY	CA	44.446	0.013	1
606	?	118	TYR	CA	56.546	0.04	1
607	?	119	LYS	CA	52.825	0.008	1
608	?	120	ARG	CA	53.680	0.003	1
609	?	121	GLU	CA	60.091	0.008	1
610	?	122	HIS	CA	59.525	0.005	1
611	?	123	ILE	CA	59.793	0.012	1
612	?	124	ASN	CA	52.777	0.005	1
613	?	125	LEU	CA	53.262	0.015	1
614	?	126	GLY	CA	44.782	0.021	1
615	?	127	CYS	CA	58.092	0.035	1
616	?	128	ASP	CA	52.383	0.041	1
617	?	129	MET	CA	54.343	0.01	1
618	?	130	ASP	CA	52.720	0.009	1
619	?	131	PHE	CA	57.802	0.006	1
620	?	132	ASP	CA	53.867	0.01	1
621	?	133	ILE	CA	63.018	0.002	1
622	?	134	ALA	CA	52.416	0.015	1
623	?	135	GLY	CA	44.292	?	1
624	?	136	PRO	CA	62.799	?	1
625	?	137	SER	CA	57.284	0.025	1
626	?	138	ILE	CA	59.536	0.01	1
627	?	139	ARG	CA	53.828	0.016	1
628	?	140	GLY	CA	43.763	0.005	1
629	?	141	ALA	CA	50.832	0.004	1
630	?	142	LEU	CA	53.627	0.003	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
631	?	143	VAL	CA	60.895	0.011	1
632	?	144	LEU	CA	51.946	0.006	1
633	?	145	GLY	CA	44.678	0.001	1
634	?	146	TYR	CA	59.074	0.009	1
635	?	147	GLU	CA	56.867	0.024	1
636	?	148	GLY	CA	45.149	0.015	1
637	?	149	TRP	CA	57.219	0.002	1
638	?	150	LEU	CA	53.472	0.02	1
639	?	151	ALA	CA	50.671	0.024	1
640	?	152	GLY	CA	45.220	0.001	1
641	?	153	TYR	CA	55.979	0.015	1
642	?	154	GLN	CA	53.066	0.0	1
643	?	155	MET	CA	52.871	0.008	1
644	?	156	ASN	CA	52.207	0.009	1
645	?	157	PHE	CA	56.117	0.003	1
646	?	158	GLU	CA	54.823	0.01	1
647	?	159	THR	CA	64.899	0.014	1
648	?	160	ALA	CA	54.424	?	1
649	?	161	LYS	CA	54.635	?	1
650	?	162	SER	CA	58.326	0.001	1
651	?	163	ARG	CA	53.672	0.029	1
652	?	164	VAL	CA	61.937	0.005	1
653	?	165	THR	CA	61.248	0.045	1
654	?	166	GLN	CA	55.286	0.005	1
655	?	167	SER	CA	57.068	0.038	1
656	?	168	ASN	CA	51.464	0.016	1
657	?	169	PHE	CA	56.028	0.002	1
658	?	170	ALA	CA	50.983	0.007	1
659	?	171	VAL	CA	60.081	0.004	1
660	?	172	GLY	CA	45.654	0.009	1
661	?	173	TYR	CA	56.470	0.012	1
662	?	174	LYS	CA	55.336	0.033	1
663	?	175	THR	CA	59.393	?	1
664	?	178	PHE	CA	56.186	0.014	1
665	?	179	GLN	CA	53.678	0.0	1
666	?	180	LEU	CA	53.483	?	1
667	?	181	HIS	CA	55.005	?	1
668	?	182	THR	CA	59.861	?	1
669	?	183	ASN	CA	52.999	0.007	1
670	?	184	VAL	CA	59.970	0.029	1
671	?	185	ASN	CA	51.254	0.004	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
672	?	186	ASP	CA	55.802	0.001	1
673	?	187	GLY	CA	45.957	0.006	1
674	?	188	THR	CA	62.465	0.003	1
675	?	189	GLU	CA	54.536	0.055	1
676	?	190	PHE	CA	55.753	0.009	1
677	?	191	GLY	CA	44.450	0.004	1
678	?	192	GLY	CA	45.452	0.018	1
679	?	193	SER	CA	56.093	0.027	1
680	?	194	ILE	CA	59.546	0.055	1
681	?	195	TYR	CA	55.552	0.017	1
682	?	196	GLN	CA	53.636	0.001	1
683	?	197	LYS	CA	55.615	0.023	1
684	?	198	VAL	CA	64.878	?	1
685	?	199	ASN	CA	51.983	?	1
686	?	202	LEU	CA	53.949	0.04	1
687	?	203	GLU	CA	54.096	0.014	1
688	?	204	THR	CA	59.357	0.012	1
689	?	205	ALA	CA	50.706	0.005	1
690	?	206	VAL	CA	59.330	0.074	1
691	?	207	ASN	CA	51.943	0.015	1
692	?	208	LEU	CA	54.098	0.01	1
693	?	209	ALA	CA	51.800	0.005	1
694	?	210	TRP	CA	57.597	0.009	1
695	?	211	THR	CA	60.303	0.002	1
696	?	212	ALA	CA	53.112	0.039	1
697	?	213	GLY	CA	44.984	0.012	1
698	?	214	ASN	CA	52.197	?	1
699	?	215	SER	CA	58.930	?	1
700	?	216	ASN	CA	52.997	0.005	1
701	?	217	THR	CA	62.561	0.019	1
702	?	218	ARG	CA	54.916	0.014	1
703	?	219	PHE	CA	55.790	0.002	1
704	?	220	GLY	CA	45.064	0.005	1
705	?	221	ILE	CA	59.549	0.018	1
706	?	222	ALA	CA	50.189	0.03	1
707	?	223	ALA	CA	50.227	0.008	1
708	?	224	LYS	CA	56.024	0.04	1
709	?	225	TYR	CA	55.144	0.044	1
710	?	226	GLN	CA	54.446	0.031	1
711	?	227	ILE	CA	64.471	0.019	1
712	?	228	ASP	CA	52.593	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
713	?	229	PRO	CA	65.456	?	1
714	?	230	ASP	CA	53.699	?	1
715	?	231	ALA	CA	51.595	0.002	1
716	?	232	CYS	CA	56.136	0.003	1
717	?	233	PHE	CA	55.419	0.049	1
718	?	234	SER	CA	57.280	0.068	1
719	?	235	ALA	CA	50.635	0.0	1
720	?	236	LYS	CA	54.565	0.011	1
721	?	237	VAL	CA	59.434	0.029	1
722	?	238	ASN	CA	50.786	0.019	1
723	?	239	ASN	CA	54.822	0.026	1
724	?	240	SER	CA	58.112	0.03	1
725	?	241	SER	CA	59.589	0.027	1
726	?	242	LEU	CA	53.681	0.018	1
727	?	243	ILE	CA	59.405	0.013	1
728	?	244	GLY	CA	44.004	0.002	1
729	?	245	LEU	CA	53.223	0.017	1
730	?	246	GLY	CA	44.584	0.009	1
731	?	247	TYR	CA	56.101	0.017	1
732	?	248	THR	CA	60.721	0.027	1
733	?	249	GLN	CA	52.355	0.084	1
734	?	254	GLY	CA	47.036	0.017	1
735	?	253	PRO	CA	62.431	?	1
736	?	255	ILE	CA	59.863	0.0	1
737	?	256	LYS	CA	54.797	0.069	1
738	?	257	LEU	CA	52.908	0.008	1
739	?	258	THR	CA	61.114	0.076	1
740	?	259	LEU	CA	52.878	0.001	1
741	?	260	SER	CA	56.733	0.015	1
742	?	261	ALA	CA	51.115	0.004	1
743	?	262	LEU	CA	52.341	0.0	1
744	?	263	LEU	CA	52.271	0.003	1
745	?	264	ASP	CA	52.261	0.006	1
746	?	265	GLY	CA	45.980	0.005	1
747	?	266	LYS	CA	56.762	0.021	1
748	?	267	ASN	CA	51.755	0.005	1
749	?	268	VAL	CA	65.056	0.017	1
750	?	269	ASN	CA	54.325	0.012	1
751	?	270	ALA	CA	51.598	0.032	1
752	?	271	GLY	CA	44.734	0.006	1
753	?	272	GLY	CA	45.522	0.001	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
754	?	273	HIS	CA	54.498	0.002	1
755	?	274	LYS	CA	54.679	0.044	1
756	?	275	LEU	CA	53.447	0.009	1
757	?	276	GLY	CA	45.063	0.081	1
758	?	277	LEU	CA	53.779	0.022	1
759	?	278	GLY	CA	44.242	0.006	1
760	?	279	LEU	CA	53.289	0.002	1
761	?	280	GLU	CA	54.003	0.005	1
762	?	281	PHE	CA	53.602	?	1
763	?	282	GLN	CA	53.883	?	1
764	?	283	ALA	CA	51.047	?	1
765	?	284	ARG	CA	55.576	?	1
766	?	285	SER	CA	56.962	?	1
767	?	101	SER	CA	56.938	?	1
768	?	5	PRO	C	174.397	?	1
769	?	6	THR	C	176.150	?	1
770	?	9	ASP	C	177.370	?	1
771	?	19	THR	C	175.275	?	1
772	?	25	GLY	C	172.849	?	1
773	?	27	ILE	C	175.093	?	1
774	?	29	LEU	C	174.365	?	1
775	?	30	ASP	C	173.854	?	1
776	?	32	LYS	C	172.072	?	1
777	?	33	THR	C	172.749	?	1
778	?	26	LEU	C	176.453	?	1
779	?	7	TYR	C	178.911	?	1
780	?	8	ALA	C	177.658	?	1
781	?	28	LYS	C	173.905	?	1
782	?	34	LYS	C	175.624	?	1
783	?	40	GLU	C	174.668	?	1
784	?	39	LEU	C	175.937	?	1
785	?	41	PHE	C	174.608	?	1
786	?	42	THR	C	173.346	?	1
787	?	43	SER	C	172.885	?	1
788	?	44	SER	C	173.100	?	1
789	?	45	GLY	C	172.056	?	1
790	?	46	SER	C	172.295	?	1
791	?	47	ALA	C	175.472	?	1
792	?	53	LYS	C	176.640	?	1
793	?	54	VAL	C	175.207	?	1
794	?	55	THR	C	172.560	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
795	?	56	GLY	C	171.366	?	1
796	?	57	SER	C	172.289	?	1
797	?	58	LEU	C	174.762	?	1
798	?	59	GLU	C	175.230	?	1
799	?	60	THR	C	171.829	?	1
800	?	61	LYS	C	174.234	?	1
801	?	62	TYR	C	173.618	?	1
802	?	66	GLU	C	176.167	?	1
803	?	67	TYR	C	173.733	?	1
804	?	68	GLY	C	175.551	?	1
805	?	69	LEU	C	176.564	?	1
806	?	70	THR	C	172.558	?	1
807	?	71	PHE	C	174.018	?	1
808	?	72	THR	C	173.599	?	1
809	?	73	VAL	C	173.643	?	1
810	?	74	LYS	C	174.101	?	1
811	?	75	TRP	C	174.677	?	1
812	?	77	THR	C	175.216	?	1
813	?	78	ASP	C	176.019	?	1
814	?	79	ASN	C	173.952	?	1
815	?	80	THR	C	173.358	?	1
816	?	81	LEU	C	175.796	?	1
817	?	82	GLY	C	172.560	?	1
818	?	83	THR	C	172.748	?	1
819	?	84	GLU	C	175.227	?	1
820	?	85	ILE	C	174.537	?	1
821	?	86	THR	C	172.990	?	1
822	?	87	VAL	C	174.470	?	1
823	?	88	GLU	C	175.436	?	1
824	?	89	ASP	C	175.287	?	1
825	?	90	GLN	C	177.311	?	1
826	?	91	LEU	C	176.785	?	1
827	?	92	ALA	C	176.282	?	1
828	?	93	ARG	C	177.265	?	1
829	?	94	GLY	C	173.832	?	1
830	?	95	LEU	C	175.281	?	1
831	?	96	LYS	C	173.968	?	1
832	?	97	LEU	C	174.697	?	1
833	?	98	THR	C	172.869	?	1
834	?	99	PHE	C	173.019	?	1
835	?	102	SER	C	173.079	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
836	?	103	PHE	C	173.525	?	1
837	?	108	GLY	C	173.776	?	1
838	?	109	LYS	C	175.923	?	1
839	?	110	LYS	C	174.951	?	1
840	?	111	ASN	C	173.490	?	1
841	?	112	ALA	C	174.871	?	1
842	?	113	LYS	C	175.363	?	1
843	?	114	ILE	C	175.014	?	1
844	?	115	LYS	C	175.836	?	1
845	?	116	THR	C	174.552	?	1
846	?	117	GLY	C	171.013	?	1
847	?	118	TYR	C	172.223	?	1
848	?	119	LYS	C	173.085	?	1
849	?	120	ARG	C	174.584	?	1
850	?	121	GLU	C	177.024	?	1
851	?	122	HIS	C	173.491	?	1
852	?	123	ILE	C	171.920	?	1
853	?	124	ASN	C	174.492	?	1
854	?	125	LEU	C	175.788	?	1
855	?	126	GLY	C	171.947	?	1
856	?	127	CYS	C	172.649	?	1
857	?	128	ASP	C	174.958	?	1
858	?	129	MET	C	173.113	?	1
859	?	130	ASP	C	175.978	?	1
860	?	131	PHE	C	174.576	?	1
861	?	133	ILE	C	176.767	?	1
862	?	134	ALA	C	177.795	?	1
863	?	136	PRO	C	177.217	?	1
864	?	137	SER	C	172.824	?	1
865	?	138	ILE	C	173.397	?	1
866	?	139	ARG	C	176.051	?	1
867	?	140	GLY	C	170.800	?	1
868	?	141	ALA	C	174.864	?	1
869	?	143	VAL	C	174.790	?	1
870	?	144	LEU	C	176.272	?	1
871	?	145	GLY	C	173.008	?	1
872	?	146	TYR	C	173.720	?	1
873	?	147	GLU	C	175.236	?	1
874	?	148	GLY	C	173.409	?	1
875	?	149	TRP	C	177.265	?	1
876	?	150	LEU	C	175.367	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
877	?	151	ALA	C	175.349	?	1
878	?	152	GLY	C	171.162	?	1
879	?	153	TYR	C	172.029	?	1
880	?	154	GLN	C	172.241	?	1
881	?	155	MET	C	174.285	?	1
882	?	156	ASN	C	173.446	?	1
883	?	157	PHE	C	173.544	?	1
884	?	158	GLU	C	177.029	?	1
885	?	159	THR	C	177.056	?	1
886	?	161	LYS	C	175.207	?	1
887	?	162	SER	C	173.033	?	1
888	?	163	ARG	C	174.444	?	1
889	?	164	VAL	C	176.959	?	1
890	?	165	THR	C	174.639	?	1
891	?	166	GLN	C	174.667	?	1
892	?	167	SER	C	172.692	?	1
893	?	168	ASN	C	171.977	?	1
894	?	169	PHE	C	173.421	?	1
895	?	170	ALA	C	176.168	?	1
896	?	171	VAL	C	175.450	?	1
897	?	172	GLY	C	170.141	?	1
898	?	173	TYR	C	173.777	?	1
899	?	174	LYS	C	173.993	?	1
900	?	177	GLU	C	173.927	?	1
901	?	178	PHE	C	174.102	?	1
902	?	179	GLN	C	173.896	?	1
903	?	182	THR	C	171.828	?	1
904	?	183	ASN	C	172.735	?	1
905	?	184	VAL	C	175.034	?	1
906	?	187	GLY	C	173.206	?	1
907	?	188	THR	C	172.537	?	1
908	?	189	GLU	C	174.267	?	1
909	?	190	PHE	C	175.606	?	1
910	?	191	GLY	C	171.677	?	1
911	?	192	GLY	C	171.504	?	1
912	?	193	SER	C	173.312	?	1
913	?	194	ILE	C	173.435	?	1
914	?	195	TYR	C	172.922	?	1
915	?	196	GLN	C	174.388	?	1
916	?	203	GLU	C	174.929	?	1
917	?	204	THR	C	171.590	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
918	?	206	VAL	C	174.404	?	1
919	?	207	ASN	C	172.556	?	1
920	?	208	LEU	C	175.342	?	1
921	?	209	ALA	C	175.338	?	1
922	?	210	TRP	C	173.330	?	1
923	?	211	THR	C	173.730	?	1
924	?	215	SER	C	174.329	?	1
925	?	216	ASN	C	174.815	?	1
926	?	217	THR	C	174.199	?	1
927	?	218	ARG	C	175.128	?	1
928	?	219	PHE	C	173.547	?	1
929	?	220	GLY	C	171.033	?	1
930	?	221	ILE	C	172.187	?	1
931	?	222	ALA	C	175.247	?	1
932	?	227	ILE	C	175.482	?	1
933	?	229	PRO	C	176.013	?	1
934	?	235	ALA	C	175.730	?	1
935	?	237	VAL	C	174.139	?	1
936	?	238	ASN	C	176.388	?	1
937	?	240	SER	C	172.793	?	1
938	?	241	SER	C	172.300	?	1
939	?	242	LEU	C	176.702	?	1
940	?	243	ILE	C	174.760	?	1
941	?	244	GLY	C	171.423	?	1
942	?	246	GLY	C	170.909	?	1
943	?	255	ILE	C	174.853	?	1
944	?	260	SER	C	172.681	?	1
945	?	261	ALA	C	173.411	?	1
946	?	262	LEU	C	175.180	?	1
947	?	263	LEU	C	175.309	?	1
948	?	264	ASP	C	176.780	?	1
949	?	265	GLY	C	173.777	?	1
950	?	266	LYS	C	177.038	?	1
951	?	267	ASN	C	175.003	?	1
952	?	268	VAL	C	177.422	?	1
953	?	269	ASN	C	175.776	?	1
954	?	270	ALA	C	177.546	?	1
955	?	271	GLY	C	174.040	?	1
956	?	272	GLY	C	174.002	?	1
957	?	273	HIS	C	176.157	?	1
958	?	274	LYS	C	175.112	?	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
959	?	276	GLY	C	171.052	?	1
960	?	277	LEU	C	175.366	?	1
961	?	278	GLY	C	171.705	?	1
962	?	279	LEU	C	174.874	?	1
963	?	282	GLN	C	174.503	?	1
964	?	284	ARG	C	174.021	?	1
965	?	101	SER	C	174.833	?	1
966	?	100	ASP	C	174.833	?	1
967	?	185	ASN	C	174.892	?	1
968	?	205	ALA	C	174.607	?	1
969	?	236	LYS	C	174.127	?	1
970	?	201	LYS	CA	56.603	?	1
971	?	201	LYS	C	175.247	?	1

7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 2986. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/1257 (0%)	0/502 (0%)	0/506 (0%)	0/249 (0%)
Sidechain	0/1454 (0%)	0/843 (0%)	0/549 (0%)	0/62 (0%)
Aromatic	0/275 (0%)	0/146 (0%)	0/122 (0%)	0/7 (0%)
Overall	0/2986 (0%)	0/1491 (0%)	0/1177 (0%)	0/318 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 3355. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/1413 (0%)	0/564 (0%)	0/570 (0%)	0/279 (0%)
Sidechain	0/1659 (0%)	0/965 (0%)	0/618 (0%)	0/76 (0%)
Aromatic	0/283 (0%)	0/150 (0%)	0/126 (0%)	0/7 (0%)
Overall	0/3355 (0%)	0/1679 (0%)	0/1314 (0%)	0/362 (0%)

7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list). RCI is only applicable to proteins.