



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:03 PM BST

PDB ID : 1OQY  
Title : Structure of the DNA repair protein hHR23a  
Authors : Walters, K.J.; Lech, P.J.; Goh, A.M.; Wang, Q.; Howley, P.M.  
Deposited on : 2003-03-11

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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

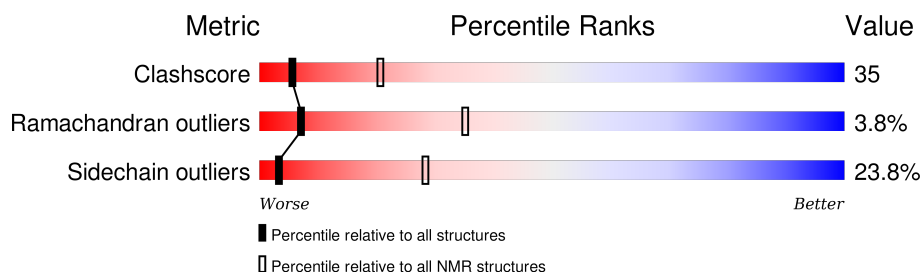
# 1 Overall quality at a glance

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  $\geq 3$ , 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	368	<div> <div>24%</div> <div>26%</div> <div>7%</div> <div>41%</div> <div>.</div> </div>

## 2 Ensemble composition and analysis

This entry contains 12 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 7 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:77 (76)	0.29	9
2	A:162-A:198 (37)	0.24	12
3	A:231-A:286 (56)	0.35	2
4	A:317-A:358 (42)	0.26	9

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. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 6, 7, 8, 10, 12
2	4, 5, 9, 11

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5484 atoms, of which 2706 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called UV excision repair protein RAD23 homolog A.

Mol	Chain	Residues	Atoms						Trace
1	A	363	Total	C	H	N	O	S	0
			5484	1725	2706	469	574	10	

There are 6 discrepancies between the modelled and reference sequences:

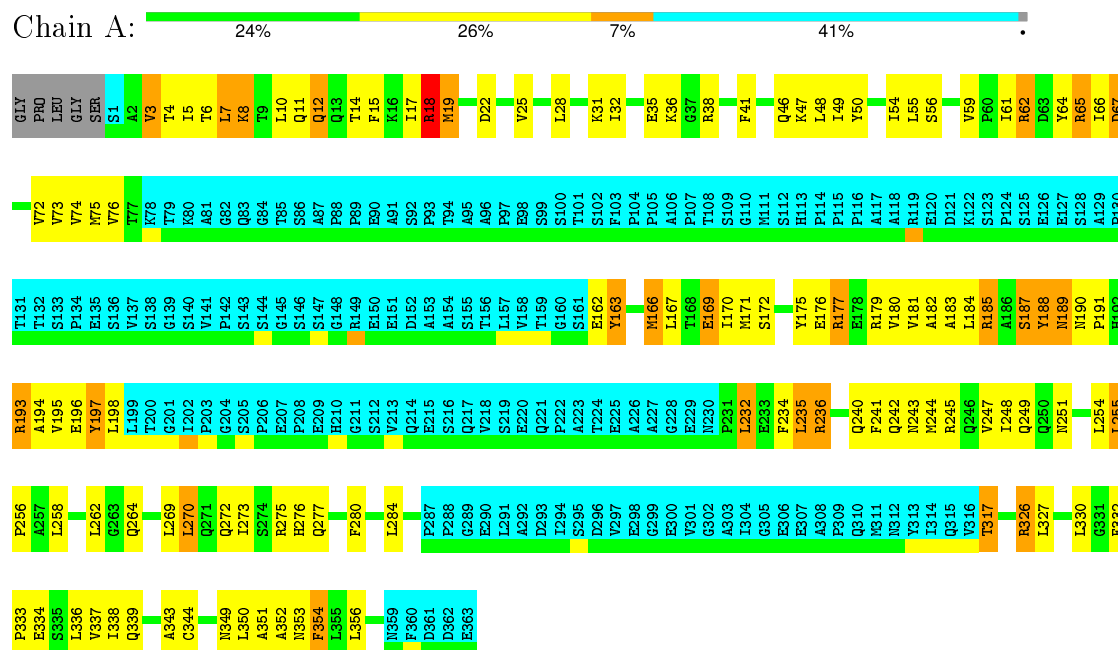
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	CLONING ARTIFACT	UNP P54725
A	-3	PRO	-	CLONING ARTIFACT	UNP P54725
A	-2	LEU	-	CLONING ARTIFACT	UNP P54725
A	-1	GLY	-	CLONING ARTIFACT	UNP P54725
A	0	SER	-	CLONING ARTIFACT	UNP P54725
A	1	SER	MET	see remark 999	UNP P54725

## 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: UV excision repair protein RAD23 homolog A

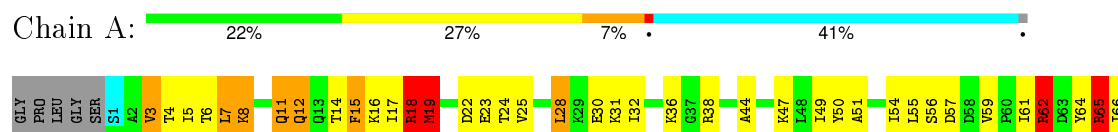


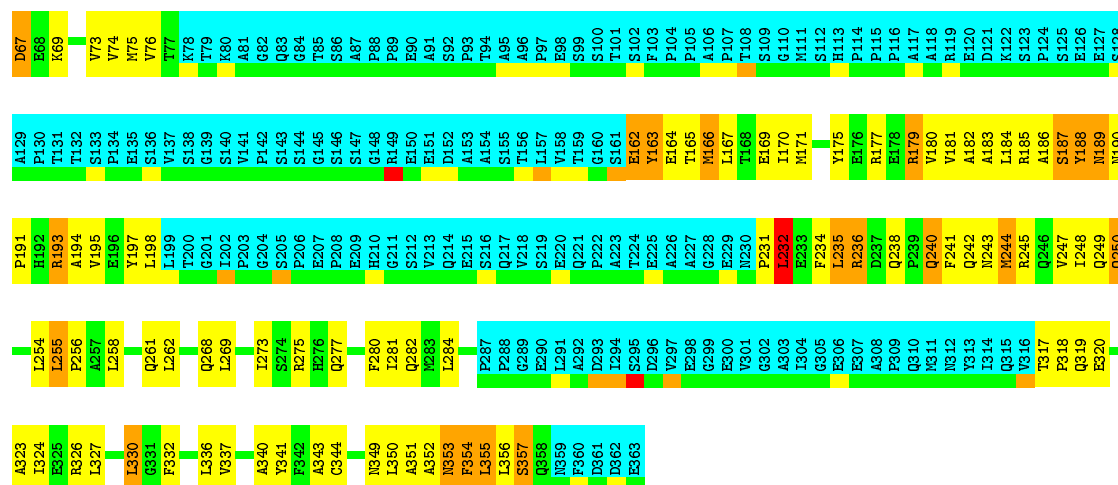
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: UV excision repair protein RAD23 homolog A

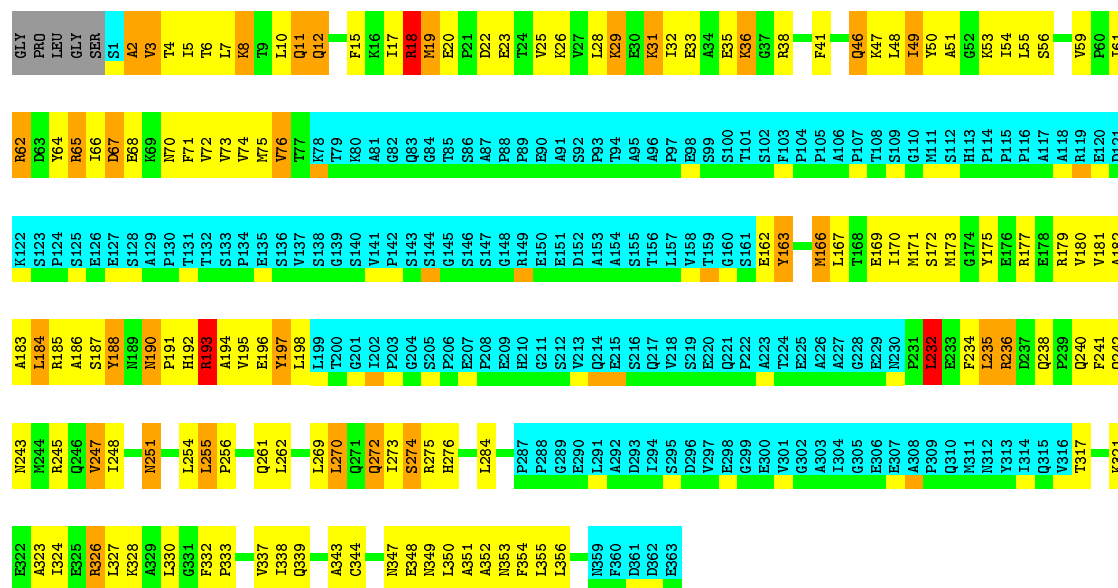




#### 4.2.2 Score per residue for model 2

- Molecule 1: UV excision repair protein RAD23 homolog A

Chain A: 21% 27% 8% 41%



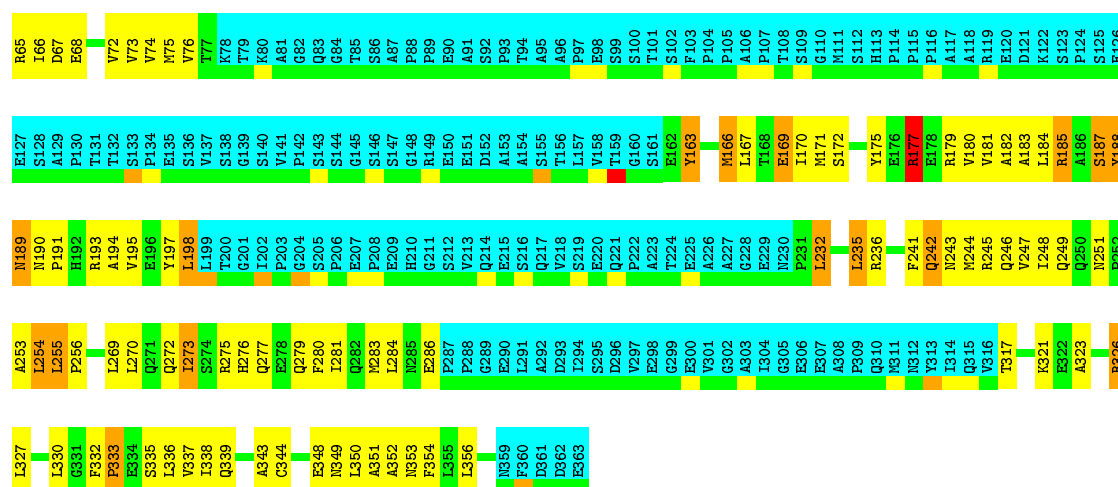
#### 4.2.3 Score per residue for model 3

- Molecule 1: UV excision repair protein RAD23 homolog A

Chain A: 23% 25% 9% 41%

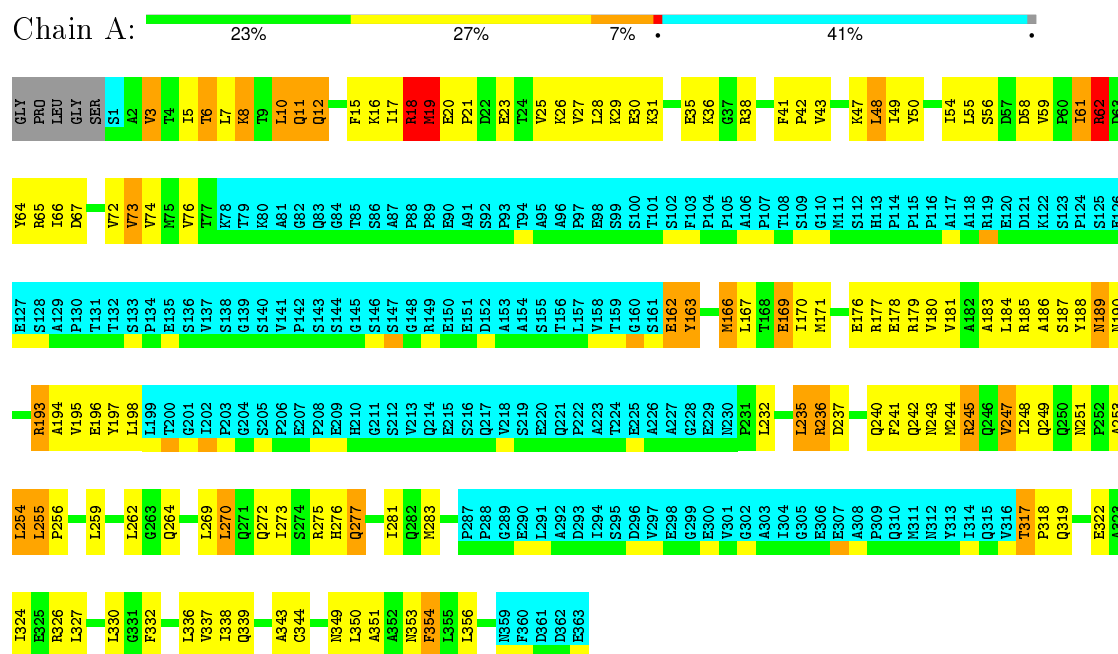






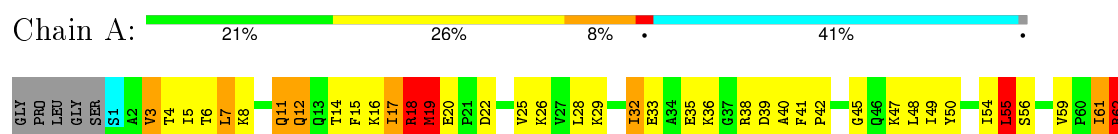
#### 4.2.6 Score per residue for model 6

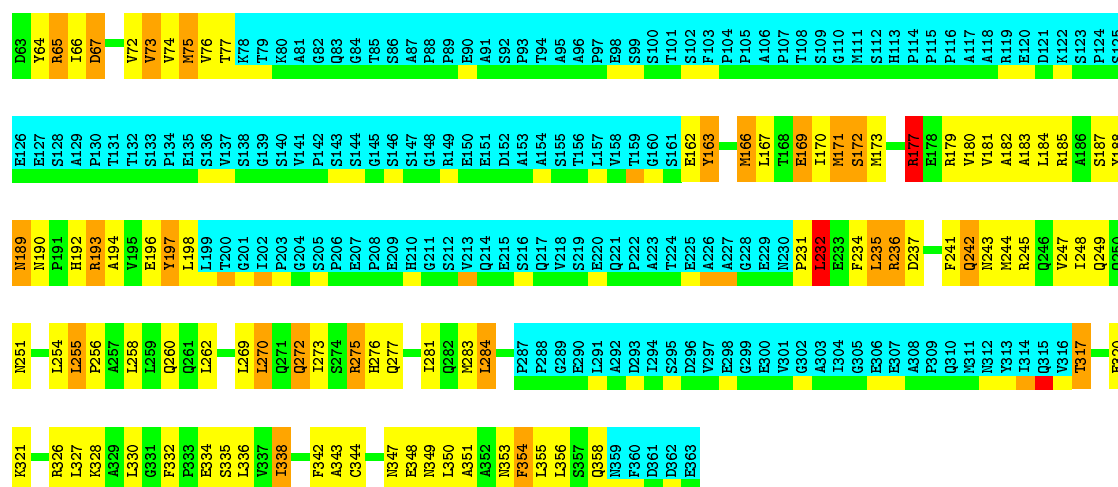
- Molecule 1: UV excision repair protein RAD23 homolog A



#### 4.2.7 Score per residue for model 7

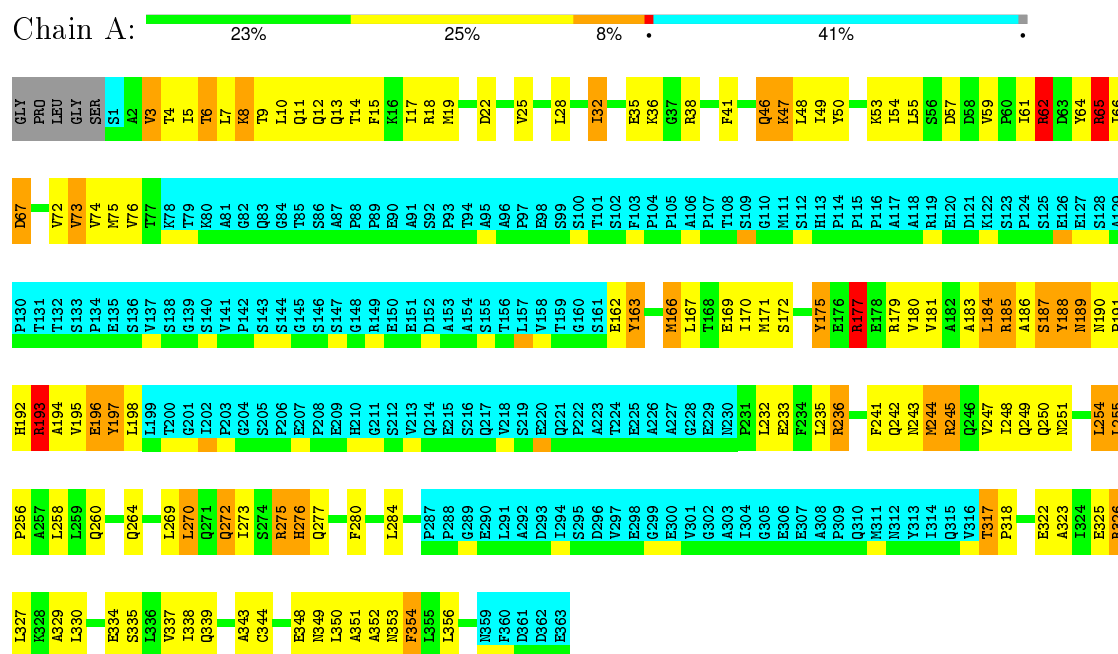
- Molecule 1: UV excision repair protein RAD23 homolog A





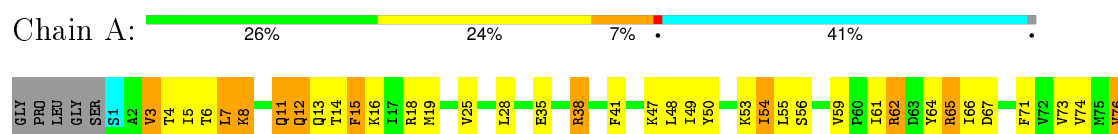
#### 4.2.8 Score per residue for model 8

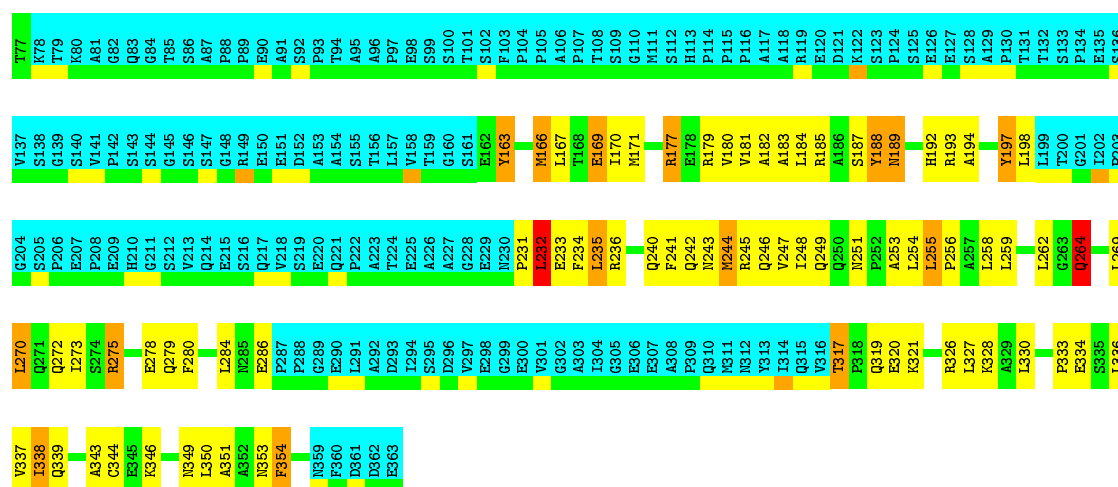
- Molecule 1: UV excision repair protein RAD23 homolog A



#### 4.2.9 Score per residue for model 9 (medoid)

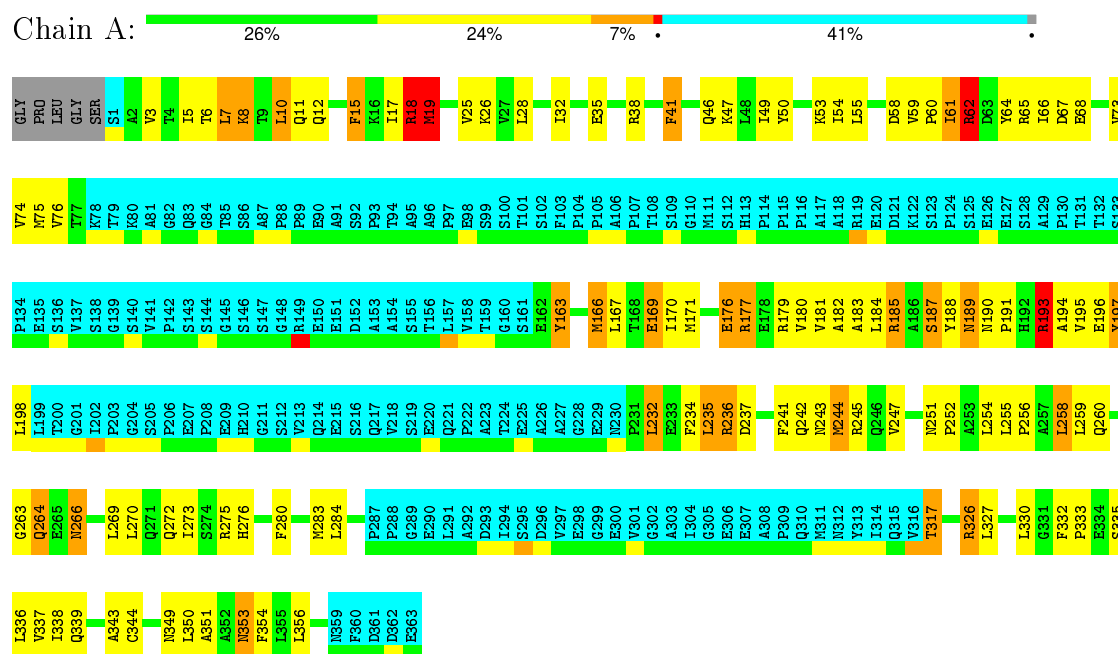
- Molecule 1: UV excision repair protein RAD23 homolog A





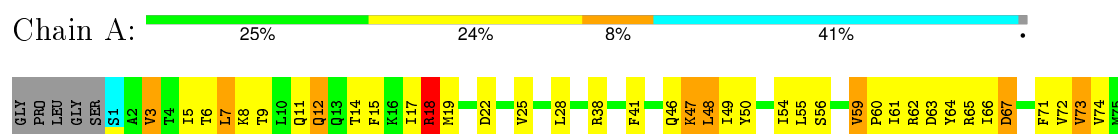
#### 4.2.10 Score per residue for model 10

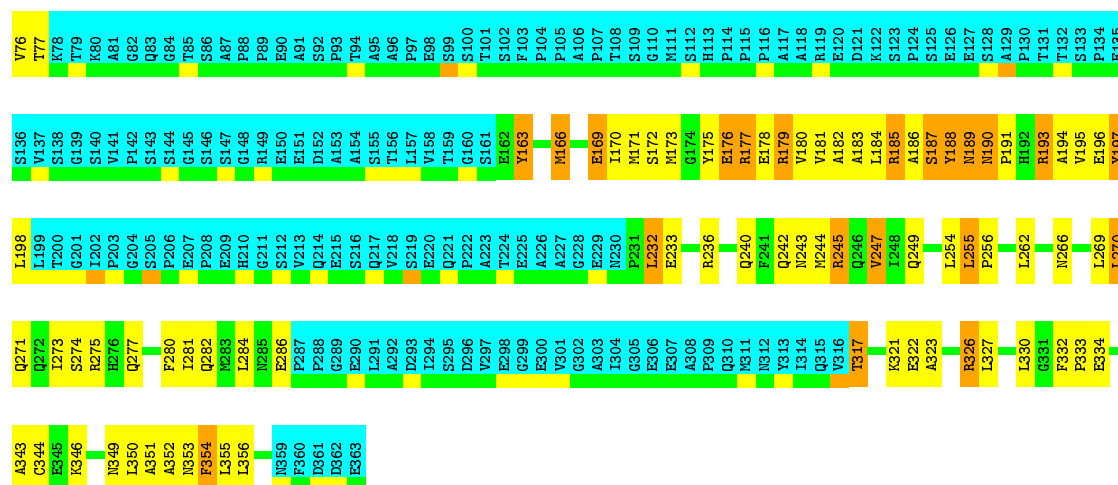
- Molecule 1: UV excision repair protein RAD23 homolog A



#### 4.2.11 Score per residue for model 11

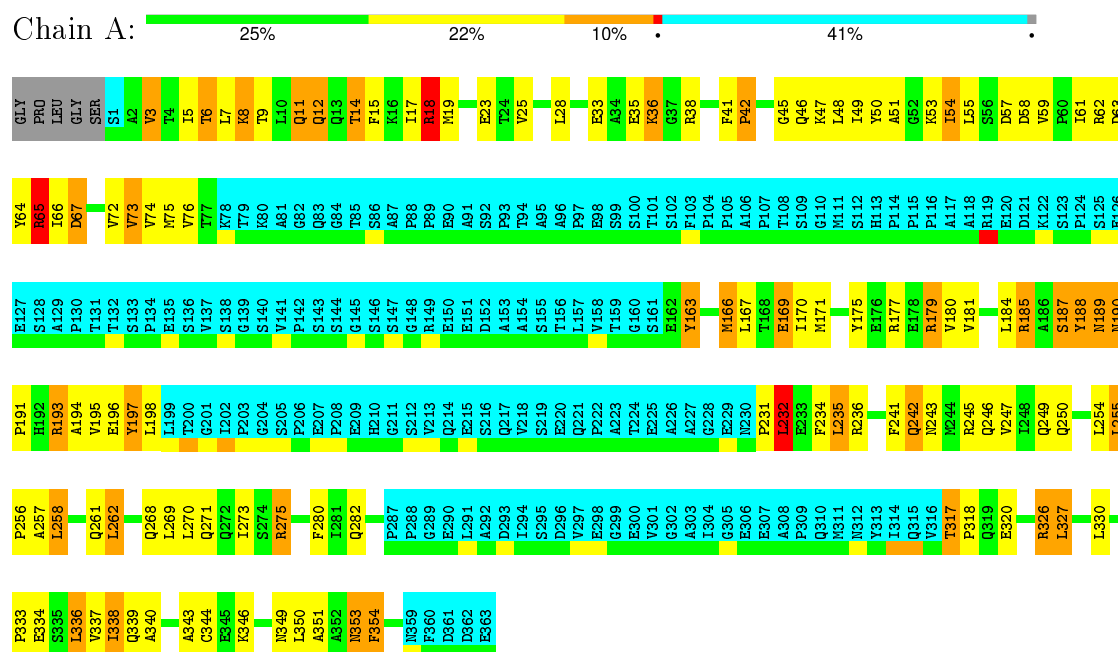
- Molecule 1: UV excision repair protein RAD23 homolog A





#### 4.2.12 Score per residue for model 12

- Molecule 1: UV excision repair protein RAD23 homolog A



## 5 Refinement protocol and experimental data overview ⓘ

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

Of the 45 calculated structures, 12 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
X-PLOR	structure solution	3.851
X-PLOR	refinement	3.851

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 [i](#)

### 6.1 Standard geometry [i](#)

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	12.0±0.0
All	All	0	144

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	236	ARG	Sidechain	12
1	A	245	ARG	Sidechain	12
1	A	18	ARG	Sidechain	12
1	A	179	ARG	Sidechain	12
1	A	38	ARG	Sidechain	12
1	A	193	ARG	Sidechain	12
1	A	275	ARG	Sidechain	12
1	A	326	ARG	Sidechain	12
1	A	62	ARG	Sidechain	12
1	A	185	ARG	Sidechain	12
1	A	177	ARG	Sidechain	12
1	A	65	ARG	Sidechain	12

### 6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1716	1740	1740	122±7
All	All	20592	20880	20880	1461

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 35.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:247:VAL:HG22	1:A:254:LEU:HD13	1.11	1.12	11	4
1:A:269:LEU:HD23	1:A:273:ILE:HD11	1.06	1.27	9	4
1:A:327:LEU:HD13	1:A:337:VAL:HG13	1.05	1.18	12	1
1:A:327:LEU:HD23	1:A:337:VAL:HG13	0.99	1.34	3	6
1:A:49:ILE:CD1	1:A:54:ILE:HG22	0.93	1.94	11	10
1:A:55:LEU:HD22	1:A:64:TYR:CG	0.91	2.01	8	8
1:A:41:PHE:CE2	1:A:76:VAL:HG21	0.89	2.03	12	3
1:A:55:LEU:HD22	1:A:64:TYR:CD1	0.88	2.02	12	10
1:A:25:VAL:HG23	1:A:59:VAL:O	0.86	1.69	12	12
1:A:170:ILE:CD1	1:A:184:LEU:HD11	0.85	2.02	9	4
1:A:269:LEU:HD23	1:A:273:ILE:HD12	0.84	1.47	8	4
1:A:176:GLU:O	1:A:180:VAL:HG23	0.83	1.72	10	1
1:A:180:VAL:O	1:A:184:LEU:HD12	0.83	1.73	8	3
1:A:334:GLU:O	1:A:338:ILE:HG22	0.82	1.74	4	4
1:A:243:ASN:O	1:A:247:VAL:HG22	0.82	1.74	9	4
1:A:61:ILE:HD13	1:A:61:ILE:O	0.82	1.74	6	2
1:A:327:LEU:HD13	1:A:337:VAL:CG1	0.82	2.05	12	1
1:A:49:ILE:HD12	1:A:54:ILE:HG22	0.82	1.47	2	1
1:A:49:ILE:HD13	1:A:54:ILE:HG22	0.81	1.51	9	8
1:A:241:PHE:CZ	1:A:284:LEU:HD22	0.81	2.09	1	1
1:A:241:PHE:CZ	1:A:284:LEU:HD12	0.81	2.11	4	3
1:A:186:ALA:HB3	1:A:197:TYR:CE2	0.80	2.12	2	4
1:A:8:LYS:O	1:A:74:VAL:HG12	0.80	1.77	8	12
1:A:180:VAL:O	1:A:184:LEU:HD13	0.79	1.78	11	6
1:A:247:VAL:HG22	1:A:254:LEU:HD23	0.79	1.52	3	1
1:A:269:LEU:CD2	1:A:273:ILE:HD11	0.79	2.08	9	3
1:A:7:LEU:HD12	1:A:15:PHE:CZ	0.77	2.15	9	6
1:A:193:ARG:O	1:A:197:TYR:N	0.77	2.17	6	3
1:A:247:VAL:CG2	1:A:254:LEU:HD13	0.77	2.04	11	2
1:A:187:SER:O	1:A:188:TYR:CB	0.77	2.32	3	9
1:A:234:PHE:CZ	1:A:235:LEU:HD12	0.77	2.14	10	2
1:A:327:LEU:HA	1:A:330:LEU:HD12	0.76	1.57	11	10
1:A:247:VAL:HG22	1:A:254:LEU:CD1	0.76	2.04	11	2
1:A:28:LEU:HD13	1:A:61:ILE:HD11	0.76	1.53	10	3

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:273:ILE:HD11	1:A:280:PHE:CG	0.75	2.16	12	1
1:A:327:LEU:HD12	1:A:337:VAL:HG13	0.74	1.55	6	1
1:A:28:LEU:HD21	1:A:48:LEU:HD21	0.74	1.60	12	4
1:A:323:ALA:O	1:A:327:LEU:HD13	0.73	1.81	1	3
1:A:170:ILE:HD12	1:A:184:LEU:HD21	0.73	1.61	12	5
1:A:330:LEU:HD21	1:A:332:PHE:CD1	0.73	2.19	1	1
1:A:343:ALA:HB2	1:A:351:ALA:HB2	0.73	1.61	8	12
1:A:248:ILE:HD11	1:A:255:LEU:HA	0.72	1.61	9	2
1:A:180:VAL:HG12	1:A:184:LEU:CD1	0.72	2.14	2	4
1:A:244:MET:O	1:A:248:ILE:HD13	0.72	1.83	9	4
1:A:180:VAL:HG12	1:A:184:LEU:HD22	0.71	1.62	10	1
1:A:180:VAL:HG12	1:A:184:LEU:HD13	0.71	1.60	2	5
1:A:49:ILE:HD11	1:A:54:ILE:HG22	0.71	1.63	3	6
1:A:197:TYR:O	1:A:197:TYR:CD1	0.71	2.44	3	4
1:A:247:VAL:HG22	1:A:254:LEU:CD2	0.71	2.16	3	1
1:A:170:ILE:HD12	1:A:184:LEU:HD11	0.70	1.61	11	4
1:A:327:LEU:CD2	1:A:337:VAL:HG13	0.70	2.17	2	4
1:A:324:ILE:HD12	1:A:337:VAL:HG12	0.70	1.62	1	3
1:A:269:LEU:HD23	1:A:273:ILE:CD1	0.70	2.11	7	4
1:A:28:LEU:CD1	1:A:61:ILE:HD11	0.69	2.16	10	3
1:A:235:LEU:HD23	1:A:241:PHE:HB2	0.69	1.63	6	4
1:A:259:LEU:HD12	1:A:263:GLY:HA3	0.69	1.64	10	1
1:A:29:LYS:HD3	1:A:43:VAL:HG13	0.69	1.63	5	1
1:A:244:MET:HB3	1:A:284:LEU:HD11	0.69	1.63	1	2
1:A:59:VAL:HG21	1:A:64:TYR:OH	0.68	1.88	8	6
1:A:231:PRO:O	1:A:232:LEU:HD12	0.68	1.88	12	5
1:A:247:VAL:HG13	1:A:254:LEU:CB	0.68	2.19	12	2
1:A:280:PHE:O	1:A:284:LEU:HD23	0.68	1.88	1	2
1:A:28:LEU:HD21	1:A:48:LEU:CD2	0.67	2.20	6	4
1:A:241:PHE:CE2	1:A:284:LEU:HD12	0.67	2.25	7	1
1:A:273:ILE:HD11	1:A:280:PHE:CD2	0.67	2.25	12	1
1:A:338:ILE:C	1:A:338:ILE:HD13	0.67	2.09	7	2
1:A:269:LEU:CD2	1:A:273:ILE:HD12	0.67	2.19	8	3
1:A:269:LEU:O	1:A:273:ILE:HG23	0.66	1.90	3	1
1:A:7:LEU:HD11	1:A:74:VAL:HG11	0.66	1.67	3	2
1:A:254:LEU:O	1:A:258:LEU:HD23	0.66	1.91	9	1
1:A:247:VAL:CG2	1:A:254:LEU:HD23	0.66	2.21	3	1
1:A:197:TYR:C	1:A:197:TYR:CD1	0.66	2.69	9	7
1:A:247:VAL:HG23	1:A:248:ILE:CD1	0.66	2.21	7	4
1:A:166:MET:HE3	1:A:169:GLU:HB3	0.65	1.67	2	1
1:A:28:LEU:HD21	1:A:48:LEU:HD11	0.65	1.68	2	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:269:LEU:O	1:A:273:ILE:HG22	0.65	1.91	10	1
1:A:188:TYR:CG	1:A:188:TYR:O	0.65	2.49	8	8
1:A:175:TYR:CZ	1:A:198:LEU:HD13	0.65	2.26	8	1
1:A:251:ASN:HB3	1:A:254:LEU:HD13	0.65	1.68	7	1
1:A:187:SER:O	1:A:188:TYR:HB2	0.65	1.91	12	7
1:A:170:ILE:HD13	1:A:184:LEU:HD11	0.65	1.69	12	9
1:A:247:VAL:HG21	1:A:258:LEU:CD2	0.65	2.21	7	3
1:A:332:PHE:CZ	1:A:356:LEU:HD21	0.65	2.27	7	4
1:A:175:TYR:CE2	1:A:198:LEU:HD13	0.64	2.27	5	2
1:A:338:ILE:HD13	1:A:338:ILE:C	0.64	2.12	4	2
1:A:188:TYR:O	1:A:188:TYR:CG	0.64	2.49	9	2
1:A:59:VAL:HG12	1:A:60:PRO:HD2	0.64	1.67	11	1
1:A:25:VAL:HG13	1:A:28:LEU:HD22	0.64	1.69	10	8
1:A:7:LEU:HB3	1:A:15:PHE:CE2	0.64	2.28	7	12
1:A:349:ASN:O	1:A:353:ASN:N	0.64	2.31	3	12
1:A:269:LEU:HD23	1:A:273:ILE:CG1	0.64	2.22	6	1
1:A:269:LEU:HD21	1:A:280:PHE:CE2	0.63	2.28	3	4
1:A:251:ASN:ND2	1:A:253:ALA:HB3	0.63	2.08	6	2
1:A:170:ILE:HD11	1:A:191:PRO:HA	0.63	1.70	2	6
1:A:194:ALA:O	1:A:198:LEU:HG	0.63	1.92	8	8
1:A:28:LEU:O	1:A:32:ILE:HD12	0.63	1.93	7	2
1:A:327:LEU:HA	1:A:330:LEU:HD23	0.62	1.69	1	1
1:A:8:LYS:HG2	1:A:73:VAL:HG22	0.62	1.70	11	2
1:A:5:ILE:N	1:A:5:ILE:HD12	0.62	2.10	5	1
1:A:183:ALA:HB2	1:A:198:LEU:HD21	0.62	1.72	6	2
1:A:55:LEU:HD13	1:A:64:TYR:CG	0.62	2.30	12	1
1:A:163:TYR:CE1	1:A:181:VAL:HG23	0.62	2.30	10	12
1:A:25:VAL:HG11	1:A:56:SER:O	0.61	1.94	5	9
1:A:61:ILE:HD11	1:A:66:ILE:HD12	0.61	1.72	8	4
1:A:349:ASN:O	1:A:350:LEU:C	0.61	2.39	1	12
1:A:163:TYR:CE1	1:A:181:VAL:CG2	0.61	2.83	4	12
1:A:6:THR:O	1:A:7:LEU:HD22	0.61	1.96	6	4
1:A:235:LEU:HD13	1:A:269:LEU:HB2	0.61	1.72	12	2
1:A:232:LEU:HD12	1:A:272:GLN:OE1	0.60	1.96	2	1
1:A:327:LEU:HD12	1:A:337:VAL:CG1	0.60	2.26	6	1
1:A:244:MET:SD	1:A:284:LEU:HD22	0.60	2.36	9	1
1:A:49:ILE:CD1	1:A:54:ILE:HD13	0.60	2.26	7	2
1:A:15:PHE:CD1	1:A:15:PHE:N	0.60	2.69	5	5
1:A:235:LEU:HD22	1:A:269:LEU:HD22	0.60	1.73	1	5
1:A:247:VAL:HG23	1:A:248:ILE:HD12	0.60	1.72	7	4
1:A:45:GLY:O	1:A:76:VAL:HA	0.59	1.97	7	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:VAL:O	1:A:73:VAL:HG12	0.59	1.97	7	5
1:A:7:LEU:HD11	1:A:48:LEU:CD1	0.59	2.27	4	1
1:A:163:TYR:CE1	1:A:167:LEU:HD22	0.59	2.32	2	7
1:A:247:VAL:HG13	1:A:254:LEU:HB3	0.59	1.73	10	2
1:A:41:PHE:CD2	1:A:76:VAL:HG21	0.59	2.33	6	3
1:A:47:LYS:HB3	1:A:54:ILE:HG23	0.59	1.75	7	2
1:A:326:ARG:C	1:A:330:LEU:HD12	0.59	2.19	10	1
1:A:15:PHE:N	1:A:15:PHE:CD1	0.58	2.70	7	6
1:A:8:LYS:CG	1:A:73:VAL:HG22	0.58	2.28	7	2
1:A:243:ASN:O	1:A:247:VAL:HG13	0.58	1.98	7	4
1:A:197:TYR:O	1:A:197:TYR:CG	0.58	2.55	3	2
1:A:11:GLN:O	1:A:12:GLN:CB	0.58	2.51	2	12
1:A:187:SER:O	1:A:188:TYR:HB3	0.58	1.98	7	4
1:A:72:VAL:HG23	1:A:72:VAL:O	0.58	1.98	12	1
1:A:163:TYR:C	1:A:163:TYR:CD1	0.58	2.77	2	8
1:A:49:ILE:HD11	1:A:54:ILE:HD13	0.58	1.74	8	2
1:A:183:ALA:O	1:A:187:SER:CB	0.58	2.51	7	4
1:A:7:LEU:HD21	1:A:32:ILE:HD11	0.58	1.73	5	1
1:A:270:LEU:HA	1:A:273:ILE:HD12	0.58	1.76	9	3
1:A:352:ALA:O	1:A:356:LEU:HD12	0.58	1.98	5	4
1:A:349:ASN:O	1:A:353:ASN:CB	0.58	2.52	5	9
1:A:269:LEU:HG	1:A:273:ILE:HD13	0.58	1.76	12	1
1:A:166:MET:HE2	1:A:184:LEU:HD21	0.57	1.75	8	5
1:A:343:ALA:HB2	1:A:351:ALA:CB	0.57	2.28	8	12
1:A:186:ALA:HB3	1:A:197:TYR:CD2	0.57	2.34	2	1
1:A:235:LEU:HD13	1:A:269:LEU:HD22	0.57	1.75	9	3
1:A:49:ILE:N	1:A:49:ILE:HD12	0.57	2.15	1	1
1:A:42:PRO:HD2	1:A:76:VAL:HG13	0.57	1.77	12	4
1:A:183:ALA:O	1:A:187:SER:OG	0.57	2.22	8	2
1:A:248:ILE:HD11	1:A:255:LEU:CA	0.57	2.29	9	3
1:A:163:TYR:CD1	1:A:163:TYR:C	0.56	2.78	11	4
1:A:20:GLU:O	1:A:61:ILE:HG21	0.56	2.00	3	3
1:A:332:PHE:CE2	1:A:355:LEU:HD22	0.56	2.35	1	1
1:A:280:PHE:CE1	1:A:284:LEU:HD11	0.56	2.35	10	1
1:A:28:LEU:HD13	1:A:61:ILE:HD13	0.56	1.76	4	2
1:A:49:ILE:O	1:A:72:VAL:HG13	0.56	2.01	5	3
1:A:269:LEU:CG	1:A:273:ILE:HD13	0.56	2.31	12	1
1:A:231:PRO:O	1:A:269:LEU:HD12	0.55	2.01	9	3
1:A:244:MET:SD	1:A:284:LEU:HD21	0.55	2.41	3	1
1:A:61:ILE:O	1:A:62:ARG:CB	0.55	2.55	10	6
1:A:5:ILE:N	1:A:5:ILE:HD13	0.55	2.17	8	3

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:LYS:HA	1:A:54:ILE:HD13	0.55	1.78	9	4
1:A:241:PHE:CE1	1:A:284:LEU:HD21	0.55	2.36	10	2
1:A:194:ALA:O	1:A:198:LEU:N	0.55	2.40	1	7
1:A:48:LEU:N	1:A:48:LEU:HD22	0.55	2.16	7	1
1:A:73:VAL:HG12	1:A:73:VAL:O	0.55	2.02	5	5
1:A:183:ALA:HA	1:A:197:TYR:CE2	0.55	2.37	2	2
1:A:23:GLU:OE2	1:A:27:VAL:HG21	0.55	2.02	6	1
1:A:197:TYR:CD1	1:A:197:TYR:N	0.54	2.73	4	1
1:A:4:THR:C	1:A:5:ILE:HD13	0.54	2.23	8	5
1:A:7:LEU:CD1	1:A:74:VAL:HG11	0.54	2.32	3	2
1:A:343:ALA:CB	1:A:351:ALA:HB2	0.54	2.33	8	12
1:A:76:VAL:O	1:A:76:VAL:HG12	0.54	2.02	6	2
1:A:247:VAL:HG21	1:A:258:LEU:HD21	0.54	1.79	7	1
1:A:235:LEU:HD13	1:A:269:LEU:HD13	0.54	1.79	10	2
1:A:334:GLU:O	1:A:338:ILE:HG23	0.54	2.03	8	1
1:A:166:MET:HE3	1:A:166:MET:CA	0.54	2.31	4	6
1:A:241:PHE:CE1	1:A:284:LEU:HD12	0.54	2.38	9	2
1:A:270:LEU:HA	1:A:273:ILE:CG2	0.54	2.33	10	4
1:A:17:ILE:HG22	1:A:18:ARG:H	0.54	1.62	10	7
1:A:191:PRO:O	1:A:195:VAL:HG22	0.54	2.02	8	1
1:A:187:SER:OG	1:A:197:TYR:CG	0.54	2.61	8	2
1:A:277:GLN:O	1:A:281:ILE:HD12	0.54	2.03	7	4
1:A:7:LEU:CB	1:A:15:PHE:CE2	0.54	2.91	12	4
1:A:280:PHE:O	1:A:284:LEU:HD12	0.54	2.03	8	1
1:A:197:TYR:O	1:A:198:LEU:C	0.53	2.46	5	1
1:A:348:GLU:O	1:A:352:ALA:HB3	0.53	2.03	8	4
1:A:4:THR:O	1:A:5:ILE:HD13	0.53	2.02	1	1
1:A:10:LEU:HD12	1:A:73:VAL:CG1	0.53	2.32	4	1
1:A:32:ILE:HD13	1:A:74:VAL:HG21	0.53	1.80	4	3
1:A:171:MET:HB2	1:A:180:VAL:HG21	0.53	1.79	10	1
1:A:11:GLN:O	1:A:12:GLN:HB2	0.53	2.03	8	2
1:A:49:ILE:CD1	1:A:54:ILE:CG2	0.53	2.85	2	1
1:A:247:VAL:HG13	1:A:248:ILE:HD12	0.53	1.81	5	1
1:A:240:GLN:HB3	1:A:262:LEU:HD21	0.53	1.81	11	2
1:A:7:LEU:HD13	1:A:72:VAL:HB	0.53	1.78	8	1
1:A:41:PHE:CD2	1:A:76:VAL:HG11	0.53	2.39	3	2
1:A:170:ILE:CD1	1:A:184:LEU:HD21	0.53	2.32	12	2
1:A:323:ALA:O	1:A:327:LEU:HD23	0.53	2.04	11	2
1:A:241:PHE:CE2	1:A:280:PHE:CE2	0.53	2.97	10	2
1:A:50:TYR:CB	1:A:55:LEU:HD11	0.53	2.34	3	4
1:A:248:ILE:HG13	1:A:255:LEU:HD12	0.53	1.79	1	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:170:ILE:CG2	1:A:180:VAL:HG13	0.52	2.34	12	4
1:A:9:THR:HG23	1:A:15:PHE:CE1	0.52	2.39	11	2
1:A:163:TYR:CE1	1:A:167:LEU:CD1	0.52	2.93	4	1
1:A:3:VAL:HG13	1:A:5:ILE:HD11	0.52	1.82	4	3
1:A:187:SER:OG	1:A:197:TYR:CB	0.52	2.57	10	2
1:A:183:ALA:HB1	1:A:197:TYR:CE2	0.52	2.39	9	1
1:A:166:MET:HE3	1:A:166:MET:O	0.52	2.05	9	4
1:A:183:ALA:O	1:A:187:SER:N	0.52	2.42	6	2
1:A:28:LEU:HD21	1:A:48:LEU:HD22	0.52	1.80	5	1
1:A:235:LEU:HD13	1:A:269:LEU:CB	0.52	2.35	12	2
1:A:3:VAL:HG13	1:A:3:VAL:O	0.52	2.05	1	6
1:A:3:VAL:O	1:A:3:VAL:HG13	0.52	2.05	2	4
1:A:180:VAL:HG12	1:A:184:LEU:CD2	0.52	2.33	10	1
1:A:55:LEU:CD2	1:A:64:TYR:CD2	0.52	2.93	5	1
1:A:28:LEU:HD12	1:A:61:ILE:HD11	0.52	1.81	12	1
1:A:247:VAL:HG21	1:A:258:LEU:HG	0.52	1.80	9	1
1:A:163:TYR:CZ	1:A:167:LEU:HD22	0.51	2.41	5	4
1:A:49:ILE:CG1	1:A:73:VAL:O	0.51	2.58	9	6
1:A:243:ASN:O	1:A:247:VAL:HG12	0.51	2.05	4	6
1:A:64:TYR:O	1:A:65:ARG:CB	0.51	2.58	12	6
1:A:48:LEU:HD13	1:A:74:VAL:HG23	0.51	1.82	8	1
1:A:183:ALA:CB	1:A:197:TYR:CE2	0.51	2.93	9	1
1:A:183:ALA:HA	1:A:197:TYR:CD2	0.51	2.40	2	1
1:A:167:LEU:HD23	1:A:180:VAL:CG1	0.51	2.36	4	1
1:A:251:ASN:ND2	1:A:254:LEU:HD13	0.51	2.21	10	1
1:A:270:LEU:HD12	1:A:270:LEU:C	0.51	2.26	9	1
1:A:251:ASN:HB3	1:A:254:LEU:HD12	0.51	1.82	8	3
1:A:166:MET:HA	1:A:169:GLU:HB2	0.51	1.81	7	11
1:A:42:PRO:CD	1:A:76:VAL:HG13	0.51	2.36	5	1
1:A:247:VAL:HB	1:A:254:LEU:HD23	0.51	1.82	7	1
1:A:187:SER:C	1:A:188:TYR:CG	0.51	2.83	2	1
1:A:270:LEU:CA	1:A:273:ILE:HD12	0.51	2.35	9	2
1:A:248:ILE:HD12	1:A:255:LEU:N	0.51	2.21	6	1
1:A:254:LEU:HD23	1:A:258:LEU:CD1	0.51	2.36	8	1
1:A:28:LEU:CD2	1:A:48:LEU:HD11	0.51	2.36	11	1
1:A:47:LYS:HB3	1:A:54:ILE:CB	0.51	2.35	6	9
1:A:32:ILE:CG2	1:A:41:PHE:CE1	0.50	2.94	5	2
1:A:251:ASN:CG	1:A:254:LEU:HD13	0.50	2.27	10	1
1:A:187:SER:OG	1:A:193:ARG:HB3	0.50	2.06	10	2
1:A:187:SER:O	1:A:193:ARG:HB3	0.50	2.06	10	1
1:A:5:ILE:HD12	1:A:5:ILE:N	0.50	2.20	7	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:166:MET:HE2	1:A:166:MET:C	0.50	2.27	10	2
1:A:10:LEU:O	1:A:10:LEU:HD23	0.50	2.06	8	1
1:A:255:LEU:N	1:A:256:PRO:HD2	0.50	2.22	9	12
1:A:170:ILE:O	1:A:173:MET:HE2	0.50	2.06	4	1
1:A:10:LEU:HD22	1:A:75:MET:HG2	0.50	1.82	4	1
1:A:50:TYR:CD1	1:A:72:VAL:HG22	0.50	2.42	2	1
1:A:166:MET:CE	1:A:184:LEU:HD21	0.50	2.36	8	2
1:A:45:GLY:O	1:A:75:MET:O	0.50	2.30	7	3
1:A:197:TYR:CD1	1:A:197:TYR:O	0.50	2.65	11	3
1:A:32:ILE:CG2	1:A:41:PHE:CD1	0.50	2.95	5	1
1:A:323:ALA:O	1:A:327:LEU:HD22	0.50	2.07	8	1
1:A:270:LEU:HA	1:A:273:ILE:HG22	0.50	1.82	8	3
1:A:332:PHE:HZ	1:A:356:LEU:HD21	0.49	1.67	7	2
1:A:324:ILE:CD1	1:A:337:VAL:HG12	0.49	2.36	1	2
1:A:17:ILE:HG22	1:A:18:ARG:N	0.49	2.22	5	6
1:A:29:LYS:CD	1:A:43:VAL:HG13	0.49	2.34	5	1
1:A:15:PHE:CD2	1:A:35:GLU:CG	0.49	2.96	6	6
1:A:187:SER:OG	1:A:197:TYR:HB2	0.49	2.08	12	1
1:A:32:ILE:HG21	1:A:41:PHE:CE1	0.49	2.42	10	1
1:A:163:TYR:HE1	1:A:167:LEU:HD13	0.49	1.67	12	5
1:A:262:LEU:C	1:A:262:LEU:HD23	0.49	2.27	11	1
1:A:163:TYR:CE1	1:A:167:LEU:HD11	0.49	2.43	4	1
1:A:50:TYR:HB2	1:A:72:VAL:HG12	0.49	1.84	12	1
1:A:234:PHE:CZ	1:A:235:LEU:HD13	0.49	2.43	2	1
1:A:243:ASN:O	1:A:247:VAL:CG2	0.49	2.61	1	5
1:A:61:ILE:HD13	1:A:61:ILE:C	0.49	2.28	6	1
1:A:195:VAL:CA	1:A:198:LEU:HD12	0.49	2.38	2	3
1:A:2:ALA:HB1	1:A:18:ARG:HD3	0.49	1.84	2	1
1:A:235:LEU:HD23	1:A:241:PHE:HD2	0.49	1.67	1	1
1:A:324:ILE:HD12	1:A:338:ILE:HA	0.49	1.85	4	1
1:A:183:ALA:CB	1:A:197:TYR:CD1	0.49	2.96	11	2
1:A:241:PHE:CD2	1:A:280:PHE:CZ	0.49	3.01	9	1
1:A:327:LEU:HB3	1:A:337:VAL:HG11	0.48	1.85	5	2
1:A:195:VAL:HA	1:A:198:LEU:HD12	0.48	1.85	2	3
1:A:54:ILE:HD12	1:A:55:LEU:O	0.48	2.08	12	1
1:A:192:HIS:O	1:A:195:VAL:HG22	0.48	2.08	2	1
1:A:163:TYR:CD1	1:A:163:TYR:O	0.48	2.66	1	1
1:A:17:ILE:HG21	1:A:31:LYS:HG2	0.48	1.85	4	4
1:A:273:ILE:CG1	1:A:280:PHE:CD2	0.48	2.96	12	1
1:A:32:ILE:CG2	1:A:41:PHE:CZ	0.48	2.96	10	1
1:A:55:LEU:HD22	1:A:64:TYR:CD2	0.48	2.43	6	2

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:264:GLN:HA	1:A:270:LEU:HD21	0.48	1.83	6	1
1:A:48:LEU:HD22	1:A:48:LEU:N	0.48	2.23	8	1
1:A:270:LEU:HD12	1:A:273:ILE:HD11	0.48	1.84	5	1
1:A:166:MET:O	1:A:166:MET:CE	0.48	2.61	3	7
1:A:193:ARG:O	1:A:197:TYR:HB3	0.48	2.08	2	2
1:A:49:ILE:HD11	1:A:54:ILE:CG2	0.48	2.35	1	1
1:A:28:LEU:HD12	1:A:32:ILE:HD11	0.48	1.84	1	1
1:A:184:LEU:O	1:A:189:ASN:CA	0.48	2.61	11	7
1:A:41:PHE:CD1	1:A:76:VAL:HG21	0.48	2.44	5	1
1:A:9:THR:HG23	1:A:15:PHE:CZ	0.48	2.43	11	1
1:A:166:MET:O	1:A:166:MET:HE3	0.48	2.08	11	1
1:A:234:PHE:CG	1:A:235:LEU:N	0.48	2.81	1	3
1:A:4:THR:HA	1:A:17:ILE:O	0.48	2.08	8	2
1:A:187:SER:O	1:A:190:ASN:ND2	0.48	2.46	2	1
1:A:332:PHE:CE2	1:A:355:LEU:HD23	0.48	2.43	2	1
1:A:54:ILE:C	1:A:54:ILE:HD12	0.48	2.29	5	2
1:A:166:MET:CE	1:A:166:MET:O	0.48	2.62	1	5
1:A:49:ILE:CG1	1:A:54:ILE:HG22	0.48	2.38	1	1
1:A:240:GLN:HG2	1:A:262:LEU:HD12	0.48	1.86	6	2
1:A:54:ILE:O	1:A:56:SER:N	0.48	2.47	7	1
1:A:352:ALA:C	1:A:356:LEU:HD12	0.48	2.29	5	5
1:A:338:ILE:HD12	1:A:339:GLN:N	0.48	2.24	2	4
1:A:188:TYR:O	1:A:189:ASN:C	0.48	2.53	5	10
1:A:317:THR:CB	1:A:318:PRO:HD2	0.48	2.39	8	4
1:A:50:TYR:HD1	1:A:72:VAL:HG22	0.48	1.68	2	1
1:A:9:THR:HG21	1:A:41:PHE:CZ	0.48	2.44	11	3
1:A:183:ALA:CB	1:A:198:LEU:HD21	0.48	2.38	6	1
1:A:251:ASN:HD22	1:A:253:ALA:HB3	0.48	1.69	9	1
1:A:7:LEU:O	1:A:15:PHE:CE1	0.47	2.67	11	2
1:A:343:ALA:HB2	1:A:351:ALA:CA	0.47	2.39	2	10
1:A:186:ALA:HB3	1:A:197:TYR:HE2	0.47	1.69	3	2
1:A:273:ILE:CD1	1:A:280:PHE:CD2	0.47	2.97	12	1
1:A:170:ILE:HD13	1:A:194:ALA:CB	0.47	2.39	11	2
1:A:269:LEU:HG	1:A:273:ILE:HG23	0.47	1.85	11	1
1:A:28:LEU:HD21	1:A:48:LEU:HG	0.47	1.86	7	1
1:A:170:ILE:HG21	1:A:198:LEU:HD11	0.47	1.85	4	3
1:A:5:ILE:CD1	1:A:5:ILE:N	0.47	2.77	5	2
1:A:167:LEU:O	1:A:171:MET:CB	0.47	2.62	4	8
1:A:197:TYR:CG	1:A:197:TYR:O	0.47	2.67	2	1
1:A:41:PHE:CE1	1:A:76:VAL:CG1	0.47	2.97	10	1
1:A:187:SER:HB2	1:A:193:ARG:C	0.47	2.30	4	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LEU:HD13	1:A:74:VAL:HB	0.47	1.85	4	1
1:A:235:LEU:HD12	1:A:269:LEU:HB2	0.47	1.84	4	1
1:A:241:PHE:CE1	1:A:284:LEU:CD1	0.47	2.98	9	2
1:A:244:MET:O	1:A:284:LEU:HD12	0.47	2.09	1	1
1:A:333:PRO:O	1:A:337:VAL:HG21	0.47	2.09	12	5
1:A:19:MET:HE3	1:A:31:LYS:HD3	0.47	1.85	5	1
1:A:181:VAL:HA	1:A:184:LEU:HB2	0.47	1.87	7	6
1:A:191:PRO:O	1:A:195:VAL:HG23	0.47	2.09	12	2
1:A:36:LYS:HG2	1:A:41:PHE:CZ	0.47	2.44	7	3
1:A:5:ILE:N	1:A:5:ILE:CD1	0.47	2.78	10	3
1:A:251:ASN:CB	1:A:254:LEU:HD13	0.47	2.39	7	1
1:A:18:ARG:O	1:A:19:MET:HG2	0.47	2.10	7	4
1:A:270:LEU:CA	1:A:273:ILE:HG22	0.47	2.39	10	1
1:A:183:ALA:O	1:A:187:SER:HB2	0.47	2.09	5	4
1:A:49:ILE:HD11	1:A:54:ILE:CD1	0.47	2.40	8	2
1:A:49:ILE:O	1:A:72:VAL:HA	0.47	2.10	5	2
1:A:170:ILE:O	1:A:171:MET:C	0.47	2.52	2	11
1:A:66:ILE:HG22	1:A:67:ASP:N	0.47	2.25	4	12
1:A:184:LEU:O	1:A:189:ASN:HB3	0.47	2.09	7	3
1:A:175:TYR:CE2	1:A:198:LEU:CD1	0.47	2.98	8	1
1:A:5:ILE:HD13	1:A:5:ILE:N	0.46	2.25	4	1
1:A:54:ILE:HG22	1:A:54:ILE:O	0.46	2.09	7	1
1:A:259:LEU:HD11	1:A:273:ILE:CG2	0.46	2.40	6	1
1:A:247:VAL:HG21	1:A:258:LEU:CG	0.46	2.40	9	1
1:A:170:ILE:HD11	1:A:191:PRO:CA	0.46	2.40	4	1
1:A:240:GLN:CB	1:A:262:LEU:HD21	0.46	2.39	3	1
1:A:187:SER:HB2	1:A:194:ALA:N	0.46	2.25	2	2
1:A:28:LEU:C	1:A:28:LEU:HD23	0.46	2.31	3	4
1:A:247:VAL:HB	1:A:254:LEU:HD13	0.46	1.87	8	2
1:A:280:PHE:CE1	1:A:284:LEU:CD1	0.46	2.98	10	2
1:A:15:PHE:CE2	1:A:35:GLU:HG2	0.46	2.46	4	4
1:A:41:PHE:CD1	1:A:76:VAL:CG1	0.46	2.99	10	1
1:A:273:ILE:HG13	1:A:274:SER:N	0.46	2.25	3	1
1:A:50:TYR:CD1	1:A:50:TYR:O	0.46	2.69	2	5
1:A:187:SER:OG	1:A:197:TYR:CD2	0.46	2.59	8	1
1:A:180:VAL:O	1:A:184:LEU:CD1	0.46	2.63	2	5
1:A:241:PHE:CZ	1:A:284:LEU:CD1	0.46	2.99	3	2
1:A:190:ASN:O	1:A:194:ALA:CB	0.46	2.64	12	4
1:A:47:LYS:HB3	1:A:54:ILE:HG21	0.46	1.88	3	1
1:A:251:ASN:CB	1:A:254:LEU:HD12	0.46	2.41	8	2
1:A:10:LEU:C	1:A:10:LEU:HD12	0.46	2.31	6	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:270:LEU:HD12	1:A:273:ILE:CD1	0.46	2.41	5	1
1:A:180:VAL:HA	1:A:198:LEU:HD21	0.46	1.87	4	1
1:A:327:LEU:CA	1:A:330:LEU:HD12	0.46	2.40	8	5
1:A:18:ARG:O	1:A:19:MET:C	0.46	2.55	4	3
1:A:36:LYS:HG3	1:A:41:PHE:CZ	0.46	2.46	12	1
1:A:350:LEU:O	1:A:354:PHE:HB3	0.46	2.11	8	6
1:A:324:ILE:HG22	1:A:328:LYS:HD3	0.46	1.87	2	1
1:A:170:ILE:CD1	1:A:195:VAL:HG23	0.46	2.41	10	1
1:A:241:PHE:CE1	1:A:284:LEU:CD2	0.46	2.99	8	1
1:A:188:TYR:CD2	1:A:190:ASN:HB2	0.45	2.45	12	8
1:A:8:LYS:CE	1:A:14:THR:OG1	0.45	2.64	11	3
1:A:61:ILE:HD11	1:A:66:ILE:CD1	0.45	2.42	11	1
1:A:194:ALA:O	1:A:198:LEU:CG	0.45	2.64	6	4
1:A:54:ILE:HD12	1:A:54:ILE:C	0.45	2.32	3	3
1:A:330:LEU:HD21	1:A:332:PHE:CE1	0.45	2.45	1	1
1:A:163:TYR:CD1	1:A:181:VAL:HG23	0.45	2.47	1	1
1:A:248:ILE:CD1	1:A:255:LEU:N	0.45	2.79	6	1
1:A:49:ILE:N	1:A:49:ILE:HD13	0.45	2.26	2	1
1:A:184:LEU:HA	1:A:187:SER:OG	0.45	2.12	2	1
1:A:193:ARG:O	1:A:194:ALA:C	0.45	2.55	6	1
1:A:28:LEU:HD23	1:A:28:LEU:C	0.45	2.32	5	4
1:A:180:VAL:C	1:A:184:LEU:HD12	0.45	2.31	8	1
1:A:54:ILE:O	1:A:54:ILE:HD12	0.45	2.11	5	2
1:A:188:TYR:O	1:A:190:ASN:N	0.45	2.50	10	8
1:A:195:VAL:N	1:A:198:LEU:HD12	0.45	2.26	2	3
1:A:184:LEU:CA	1:A:189:ASN:HA	0.45	2.42	8	4
1:A:19:MET:HG3	1:A:20:GLU:N	0.45	2.27	6	1
1:A:183:ALA:O	1:A:187:SER:HB3	0.45	2.12	4	1
1:A:270:LEU:HD13	1:A:273:ILE:HD11	0.45	1.87	11	1
1:A:183:ALA:HA	1:A:197:TYR:OH	0.45	2.11	9	1
1:A:48:LEU:HD23	1:A:72:VAL:HG11	0.45	1.89	11	1
1:A:332:PHE:CE1	1:A:355:LEU:CD2	0.45	3.00	11	1
1:A:235:LEU:HD23	1:A:241:PHE:CD2	0.45	2.47	1	1
1:A:17:ILE:HG23	1:A:35:GLU:OE1	0.45	2.12	7	1
1:A:49:ILE:HB	1:A:73:VAL:O	0.45	2.12	1	3
1:A:244:MET:HG3	1:A:258:LEU:HD12	0.45	1.88	10	1
1:A:167:LEU:HD12	1:A:184:LEU:HD22	0.45	1.88	7	1
1:A:48:LEU:HB2	1:A:55:LEU:HB2	0.45	1.88	8	1
1:A:4:THR:C	1:A:5:ILE:HD12	0.45	2.32	5	2
1:A:49:ILE:N	1:A:49:ILE:CD1	0.45	2.79	1	1
1:A:47:LYS:HD3	1:A:54:ILE:HG21	0.45	1.88	5	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LEU:HB3	1:A:15:PHE:CD2	0.45	2.47	10	4
1:A:55:LEU:CD2	1:A:64:TYR:CD1	0.44	2.99	6	4
1:A:49:ILE:O	1:A:73:VAL:N	0.44	2.50	7	1
1:A:325:GLU:O	1:A:329:ALA:HB2	0.44	2.12	8	1
1:A:14:THR:C	1:A:15:PHE:CD1	0.44	2.91	12	2
1:A:332:PHE:HE2	1:A:355:LEU:HD13	0.44	1.73	1	1
1:A:269:LEU:O	1:A:273:ILE:HG12	0.44	2.12	5	1
1:A:59:VAL:HG12	1:A:63:ASP:HB3	0.44	1.88	12	1
1:A:47:LYS:HB3	1:A:54:ILE:HB	0.44	1.89	6	1
1:A:7:LEU:HG	1:A:17:ILE:HD11	0.44	1.89	3	1
1:A:8:LYS:O	1:A:74:VAL:N	0.44	2.50	4	7
1:A:15:PHE:CD2	1:A:35:GLU:HG2	0.44	2.48	8	3
1:A:183:ALA:CA	1:A:197:TYR:OH	0.44	2.66	9	1
1:A:25:VAL:CG1	1:A:28:LEU:HD22	0.44	2.41	10	2
1:A:167:LEU:HD23	1:A:180:VAL:HG12	0.44	1.88	4	1
1:A:15:PHE:CE2	1:A:35:GLU:CD	0.44	2.91	3	1
1:A:255:LEU:CB	1:A:256:PRO:CD	0.44	2.96	6	3
1:A:327:LEU:HD23	1:A:337:VAL:CG1	0.44	2.37	9	2
1:A:176:GLU:O	1:A:180:VAL:HG21	0.44	2.13	11	2
1:A:320:GLU:CB	1:A:341:TYR:CE2	0.44	3.00	1	1
1:A:10:LEU:HD12	1:A:75:MET:HG2	0.44	1.89	10	1
1:A:242:GLN:N	1:A:242:GLN:NE2	0.44	2.66	5	1
1:A:7:LEU:HD23	1:A:17:ILE:HG13	0.44	1.89	3	1
1:A:166:MET:CA	1:A:166:MET:HE3	0.44	2.43	12	1
1:A:28:LEU:HD21	1:A:48:LEU:CD1	0.44	2.42	6	1
1:A:243:ASN:O	1:A:247:VAL:CG1	0.44	2.66	3	6
1:A:183:ALA:CB	1:A:198:LEU:CD2	0.44	2.96	1	2
1:A:50:TYR:CZ	1:A:66:ILE:HA	0.44	2.47	9	7
1:A:181:VAL:HG13	1:A:182:ALA:N	0.44	2.28	2	2
1:A:272:GLN:O	1:A:276:HIS:N	0.44	2.51	8	5
1:A:324:ILE:HD13	1:A:324:ILE:N	0.44	2.28	4	1
1:A:5:ILE:N	1:A:17:ILE:O	0.44	2.51	6	2
1:A:187:SER:O	1:A:193:ARG:CB	0.44	2.66	7	1
1:A:175:TYR:CZ	1:A:198:LEU:CD1	0.44	2.99	8	1
1:A:277:GLN:HG2	1:A:281:ILE:HD11	0.43	1.90	6	1
1:A:240:GLN:HB3	1:A:262:LEU:HD22	0.43	1.88	9	1
1:A:7:LEU:O	1:A:15:PHE:CD1	0.43	2.71	5	2
1:A:272:GLN:NE2	1:A:276:HIS:CE1	0.43	2.86	2	1
1:A:195:VAL:HG23	1:A:196:GLU:N	0.43	2.28	8	1
1:A:71:PHE:O	1:A:71:PHE:CD1	0.43	2.71	11	1
1:A:18:ARG:O	1:A:19:MET:CG	0.43	2.66	4	2

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ILE:HG21	1:A:46:GLN:OE1	0.43	2.14	8	1
1:A:240:GLN:HA	1:A:262:LEU:HD11	0.43	1.90	4	1
1:A:270:LEU:HA	1:A:273:ILE:HG12	0.43	1.89	3	1
1:A:17:ILE:O	1:A:19:MET:N	0.43	2.52	3	1
1:A:270:LEU:O	1:A:273:ILE:HG12	0.43	2.12	3	1
1:A:270:LEU:HA	1:A:273:ILE:CG1	0.43	2.42	11	1
1:A:23:GLU:H	1:A:61:ILE:HG22	0.43	1.74	1	1
1:A:184:LEU:O	1:A:189:ASN:CB	0.43	2.67	7	2
1:A:264:GLN:HA	1:A:270:LEU:HD11	0.43	1.89	10	1
1:A:48:LEU:O	1:A:55:LEU:N	0.43	2.51	7	1
1:A:197:TYR:CD1	1:A:197:TYR:C	0.43	2.91	6	1
1:A:324:ILE:HG21	1:A:338:ILE:HG22	0.43	1.90	6	1
1:A:269:LEU:C	1:A:273:ILE:HG22	0.43	2.33	10	1
1:A:40:ALA:O	1:A:76:VAL:HG11	0.43	2.14	7	2
1:A:332:PHE:N	1:A:332:PHE:CD1	0.43	2.87	6	3
1:A:28:LEU:CD1	1:A:61:ILE:HD13	0.43	2.41	4	1
1:A:54:ILE:O	1:A:54:ILE:HG22	0.43	2.14	8	1
1:A:181:VAL:CG1	1:A:182:ALA:N	0.43	2.82	10	7
1:A:247:VAL:CG1	1:A:248:ILE:HD12	0.43	2.44	4	2
1:A:247:VAL:HG13	1:A:254:LEU:HB2	0.43	1.89	12	1
1:A:167:LEU:HD11	1:A:180:VAL:HB	0.43	1.89	9	3
1:A:241:PHE:CE2	1:A:280:PHE:CZ	0.43	3.07	9	1
1:A:47:LYS:HB3	1:A:54:ILE:CG2	0.43	2.44	5	2
1:A:41:PHE:CE1	1:A:76:VAL:CG2	0.43	3.01	5	1
1:A:352:ALA:O	1:A:355:LEU:N	0.43	2.52	3	1
1:A:234:PHE:CZ	1:A:268:GLN:CB	0.43	3.02	12	1
1:A:317:THR:HB	1:A:318:PRO:HD2	0.43	1.89	1	1
1:A:47:LYS:O	1:A:74:VAL:HA	0.42	2.14	5	2
1:A:163:TYR:CE1	1:A:167:LEU:HG	0.42	2.49	4	1
1:A:187:SER:HB2	1:A:193:ARG:CB	0.42	2.44	4	1
1:A:10:LEU:HD23	1:A:10:LEU:O	0.42	2.13	2	1
1:A:171:MET:CB	1:A:180:VAL:HG21	0.42	2.43	10	1
1:A:36:LYS:HG2	1:A:41:PHE:CE2	0.42	2.50	5	1
1:A:166:MET:CA	1:A:166:MET:CE	0.42	2.97	12	1
1:A:184:LEU:O	1:A:189:ASN:OD1	0.42	2.37	4	1
1:A:166:MET:HA	1:A:166:MET:HE3	0.42	1.92	4	1
1:A:54:ILE:O	1:A:54:ILE:CG1	0.42	2.66	1	1
1:A:320:GLU:HB2	1:A:341:TYR:CE2	0.42	2.50	1	1
1:A:194:ALA:O	1:A:197:TYR:N	0.42	2.53	4	1
1:A:183:ALA:HB2	1:A:197:TYR:CE1	0.42	2.49	11	1
1:A:330:LEU:HD11	1:A:332:PHE:CD1	0.42	2.49	1	1

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LEU:O	1:A:14:THR:HG23	0.42	2.15	1	1
1:A:194:ALA:O	1:A:198:LEU:CB	0.42	2.67	1	1
1:A:270:LEU:HD22	1:A:273:ILE:HD12	0.42	1.90	6	1
1:A:273:ILE:CG2	1:A:280:PHE:CD2	0.42	3.03	5	1
1:A:3:VAL:HG21	1:A:62:ARG:NH1	0.42	2.30	3	1
1:A:25:VAL:O	1:A:28:LEU:CB	0.42	2.67	1	1
1:A:55:LEU:HG	1:A:64:TYR:CD2	0.42	2.49	7	1
1:A:327:LEU:N	1:A:327:LEU:CD1	0.42	2.82	8	1
1:A:187:SER:CB	1:A:194:ALA:N	0.42	2.83	2	1
1:A:191:PRO:O	1:A:195:VAL:CG2	0.42	2.67	5	3
1:A:273:ILE:CG2	1:A:274:SER:N	0.42	2.83	4	2
1:A:7:LEU:CD2	1:A:32:ILE:HD11	0.42	2.43	5	1
1:A:258:LEU:HD13	1:A:262:LEU:HB2	0.42	1.91	12	1
1:A:50:TYR:CG	1:A:50:TYR:O	0.42	2.72	12	1
1:A:10:LEU:CD1	1:A:73:VAL:CG1	0.42	2.97	4	1
1:A:338:ILE:CD1	1:A:338:ILE:C	0.42	2.84	4	1
1:A:25:VAL:HB	1:A:57:ASP:HA	0.42	1.92	1	3
1:A:23:GLU:O	1:A:61:ILE:HG12	0.42	2.15	12	1
1:A:258:LEU:CD1	1:A:262:LEU:CB	0.42	2.97	12	1
1:A:336:LEU:O	1:A:340:ALA:CB	0.42	2.68	12	2
1:A:71:PHE:CD1	1:A:71:PHE:O	0.42	2.73	2	2
1:A:269:LEU:O	1:A:273:ILE:N	0.42	2.53	10	1
1:A:48:LEU:N	1:A:48:LEU:CD2	0.42	2.83	7	1
1:A:48:LEU:HB3	1:A:72:VAL:HG11	0.42	1.90	7	1
1:A:178:GLU:O	1:A:181:VAL:HG12	0.42	2.15	6	1
1:A:240:GLN:CB	1:A:262:LEU:HD22	0.42	2.45	9	1
1:A:173:MET:HB3	1:A:175:TYR:CE2	0.41	2.50	11	1
1:A:255:LEU:HB3	1:A:256:PRO:HD3	0.41	1.91	10	1
1:A:247:VAL:HB	1:A:254:LEU:HD22	0.41	1.92	9	1
1:A:242:GLN:NE2	1:A:242:GLN:N	0.41	2.68	3	3
1:A:49:ILE:N	1:A:73:VAL:O	0.41	2.53	2	1
1:A:326:ARG:O	1:A:330:LEU:N	0.41	2.53	10	1
1:A:255:LEU:HD23	1:A:255:LEU:C	0.41	2.35	10	1
1:A:18:ARG:O	1:A:19:MET:O	0.41	2.37	6	1
1:A:317:THR:HG22	1:A:318:PRO:HD2	0.41	1.92	8	2
1:A:280:PHE:CD1	1:A:280:PHE:C	0.41	2.93	9	1
1:A:332:PHE:CE2	1:A:355:LEU:HD13	0.41	2.50	1	1
1:A:7:LEU:HD13	1:A:8:LYS:N	0.41	2.30	9	2
1:A:28:LEU:HD23	1:A:29:LYS:N	0.41	2.31	6	1
1:A:29:LYS:CE	1:A:43:VAL:HG13	0.41	2.45	6	1
1:A:21:PRO:O	1:A:62:ARG:HB2	0.41	2.15	6	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LYS:O	1:A:35:GLU:CB	0.41	2.69	3	1
1:A:50:TYR:CB	1:A:55:LEU:CD1	0.41	2.99	7	1
1:A:187:SER:O	1:A:188:TYR:CD2	0.41	2.74	2	1
1:A:8:LYS:NZ	1:A:14:THR:OG1	0.41	2.53	7	1
1:A:54:ILE:O	1:A:54:ILE:HG13	0.41	2.16	9	1
1:A:350:LEU:N	1:A:350:LEU:CD2	0.41	2.84	8	3
1:A:7:LEU:HB2	1:A:15:PHE:CE2	0.41	2.51	12	2
1:A:266:ASN:O	1:A:266:ASN:ND2	0.41	2.54	10	1
1:A:254:LEU:HD23	1:A:258:LEU:HD11	0.41	1.90	8	1
1:A:170:ILE:HG21	1:A:180:VAL:HG13	0.41	1.92	12	1
1:A:59:VAL:CG1	1:A:60:PRO:HD2	0.41	2.46	10	1
1:A:166:MET:O	1:A:166:MET:HE2	0.41	2.15	10	1
1:A:255:LEU:N	1:A:256:PRO:CD	0.41	2.84	10	1
1:A:187:SER:HB2	1:A:193:ARG:HB3	0.41	1.92	6	1
1:A:184:LEU:O	1:A:189:ASN:N	0.41	2.53	9	1
1:A:55:LEU:HD23	1:A:64:TYR:CD2	0.41	2.51	5	1
1:A:166:MET:CE	1:A:166:MET:CA	0.41	2.99	4	1
1:A:258:LEU:CD1	1:A:258:LEU:N	0.41	2.83	4	1
1:A:352:ALA:O	1:A:353:ASN:C	0.41	2.59	3	1
1:A:188:TYR:O	1:A:188:TYR:CD1	0.41	2.74	12	1
1:A:247:VAL:HG22	1:A:254:LEU:HB3	0.41	1.93	12	1
1:A:72:VAL:CG2	1:A:72:VAL:O	0.41	2.68	12	1
1:A:257:ALA:O	1:A:261:GLN:CG	0.41	2.68	12	1
1:A:48:LEU:CD2	1:A:72:VAL:HG11	0.41	2.46	11	1
1:A:320:GLU:OE1	1:A:342:PHE:CZ	0.41	2.73	7	1
1:A:163:TYR:CE1	1:A:167:LEU:HD13	0.41	2.50	8	1
1:A:338:ILE:HD13	1:A:339:GLN:N	0.41	2.30	9	1
1:A:194:ALA:O	1:A:195:VAL:C	0.41	2.57	4	2
1:A:190:ASN:OD1	1:A:192:HIS:CD2	0.41	2.74	2	1
1:A:36:LYS:CG	1:A:41:PHE:CZ	0.41	3.04	7	1
1:A:259:LEU:O	1:A:264:GLN:HB2	0.41	2.16	9	1
1:A:327:LEU:HD12	1:A:330:LEU:HD12	0.40	1.92	3	1
1:A:254:LEU:O	1:A:258:LEU:HB2	0.40	2.15	12	1
1:A:258:LEU:HD13	1:A:262:LEU:CB	0.40	2.46	12	1
1:A:29:LYS:HA	1:A:32:ILE:HD12	0.40	1.92	2	1
1:A:197:TYR:C	1:A:197:TYR:HD1	0.40	2.18	10	1
1:A:252:PRO:O	1:A:256:PRO:CD	0.40	2.69	10	1
1:A:338:ILE:C	1:A:338:ILE:CD1	0.40	2.86	9	1
1:A:166:MET:HE1	1:A:170:ILE:HD12	0.40	1.93	5	1
1:A:241:PHE:C	1:A:241:PHE:CD1	0.40	2.94	5	1
1:A:241:PHE:CD1	1:A:241:PHE:C	0.40	2.94	3	1

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:240:GLN:CG	1:A:262:LEU:HD21	0.40	2.46	3	1
1:A:351:ALA:O	1:A:354:PHE:CD2	0.40	2.74	1	1
1:A:15:PHE:CD2	1:A:35:GLU:HG3	0.40	2.51	10	1
1:A:170:ILE:HG22	1:A:180:VAL:HG13	0.40	1.92	8	1
1:A:183:ALA:CA	1:A:197:TYR:CE2	0.40	3.04	9	1
1:A:46:GLN:HA	1:A:75:MET:O	0.40	2.17	12	2
1:A:234:PHE:CE2	1:A:268:GLN:OE1	0.40	2.75	1	1
1:A:255:LEU:HB3	1:A:256:PRO:CD	0.40	2.47	10	1
1:A:49:ILE:CD1	1:A:54:ILE:CD1	0.40	2.99	7	1
1:A:167:LEU:HD11	1:A:181:VAL:N	0.40	2.32	7	1
1:A:244:MET:O	1:A:248:ILE:CG1	0.40	2.69	6	1
1:A:317:THR:CB	1:A:318:PRO:CD	0.40	2.99	8	1
1:A:7:LEU:HD11	1:A:48:LEU:HD12	0.40	1.91	4	1
1:A:73:VAL:CG1	1:A:73:VAL:O	0.40	2.70	11	1
1:A:327:LEU:CB	1:A:337:VAL:HG11	0.40	2.46	8	1
1:A:325:GLU:HG3	1:A:326:ARG:N	0.40	2.31	8	1
1:A:163:TYR:O	1:A:163:TYR:CD1	0.40	2.75	3	1
1:A:167:LEU:O	1:A:171:MET:HB2	0.40	2.17	2	1
1:A:75:MET:C	1:A:76:VAL:HG13	0.40	2.36	2	1
1:A:171:MET:O	1:A:172:SER:C	0.40	2.60	7	1
1:A:188:TYR:CD2	1:A:193:ARG:HB2	0.40	2.52	6	1
1:A:270:LEU:HD12	1:A:270:LEU:O	0.40	2.16	9	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	211/368 (57%)	171±4 (81±2%)	32±3 (15±1%)	8±2 (4±1%)	7	35
All	All	2532/4416 (57%)	2053 (81%)	382 (15%)	97 (4%)	7	35

All 24 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	3	VAL	12
1	A	232	LEU	12
1	A	189	ASN	9
1	A	22	ASP	8
1	A	188	TYR	7
1	A	19	MET	7
1	A	76	VAL	7
1	A	73	VAL	5
1	A	333	PRO	5
1	A	177	ARG	4
1	A	51	ALA	3
1	A	264	GLN	2
1	A	334	GLU	2
1	A	18	ARG	2
1	A	175	TYR	2
1	A	2	ALA	2
1	A	42	PRO	1
1	A	176	GLU	1
1	A	192	HIS	1
1	A	162	GLU	1
1	A	250	GLN	1
1	A	17	ILE	1
1	A	55	LEU	1
1	A	198	LEU	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	188/311 (60%)	143±4 (76±2%)	45±4 (24±2%)	3	28
All	All	2256/3732 (60%)	1718 (76%)	538 (24%)	3	28

All 128 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	242	GLN	12
1	A	344	CYS	12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	354	PHE	12
1	A	166	MET	12
1	A	163	TYR	12
1	A	317	THR	11
1	A	235	LEU	11
1	A	6	THR	11
1	A	255	LEU	11
1	A	232	LEU	10
1	A	12	GLN	9
1	A	270	LEU	9
1	A	19	MET	9
1	A	249	GLN	9
1	A	8	LYS	9
1	A	244	MET	8
1	A	18	ARG	8
1	A	169	GLU	8
1	A	236	ARG	8
1	A	67	ASP	8
1	A	172	SER	7
1	A	7	LEU	7
1	A	187	SER	7
1	A	197	TYR	7
1	A	185	ARG	7
1	A	62	ARG	7
1	A	193	ARG	6
1	A	26	LYS	6
1	A	11	GLN	6
1	A	336	LEU	6
1	A	16	LYS	6
1	A	283	MET	5
1	A	247	VAL	5
1	A	162	GLU	5
1	A	36	LYS	5
1	A	177	ARG	5
1	A	321	LYS	5
1	A	246	GLN	5
1	A	53	LYS	5
1	A	275	ARG	5
1	A	272	GLN	5
1	A	250	GLN	5
1	A	65	ARG	5
1	A	75	MET	5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	326	ARG	5
1	A	338	ILE	4
1	A	282	GLN	4
1	A	322	GLU	4
1	A	61	ILE	4
1	A	286	GLU	4
1	A	319	GLN	4
1	A	46	GLN	4
1	A	13	GLN	4
1	A	196	GLU	4
1	A	33	GLU	4
1	A	245	ARG	4
1	A	335	SER	4
1	A	15	PHE	4
1	A	233	GLU	4
1	A	192	HIS	4
1	A	277	GLN	4
1	A	10	LEU	3
1	A	353	ASN	3
1	A	58	ASP	3
1	A	29	LYS	3
1	A	237	ASP	3
1	A	264	GLN	3
1	A	254	LEU	3
1	A	68	GLU	3
1	A	260	GLN	3
1	A	179	ARG	3
1	A	31	LYS	3
1	A	258	LEU	3
1	A	190	ASN	3
1	A	339	GLN	3
1	A	48	LEU	3
1	A	262	LEU	3
1	A	346	LYS	3
1	A	38	ARG	3
1	A	39	ASP	3
1	A	279	GLN	2
1	A	355	LEU	2
1	A	251	ASN	2
1	A	176	GLU	2
1	A	54	ILE	2
1	A	173	MET	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	328	LYS	2
1	A	14	THR	2
1	A	30	GLU	2
1	A	189	ASN	2
1	A	266	ASN	2
1	A	55	LEU	2
1	A	240	GLN	2
1	A	23	GLU	2
1	A	238	GLN	2
1	A	274	SER	2
1	A	47	LYS	2
1	A	261	GLN	2
1	A	284	LEU	2
1	A	347	ASN	2
1	A	41	PHE	2
1	A	271	GLN	2
1	A	69	LYS	2
1	A	320	GLU	2
1	A	32	ILE	2
1	A	276	HIS	2
1	A	184	LEU	2
1	A	22	ASP	2
1	A	77	THR	1
1	A	63	ASP	1
1	A	59	VAL	1
1	A	348	GLU	1
1	A	357	SER	1
1	A	243	ASN	1
1	A	188	TYR	1
1	A	171	MET	1
1	A	49	ILE	1
1	A	24	THR	1
1	A	28	LEU	1
1	A	70	ASN	1
1	A	327	LEU	1
1	A	17	ILE	1
1	A	330	LEU	1
1	A	5	ILE	1
1	A	278	GLU	1
1	A	269	LEU	1
1	A	178	GLU	1
1	A	273	ILE	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