Full wwPDB NMR Structure Validation Report (i)

Jun 16, 2024 – 04:26 AM EDT

PDB ID	:	2L3R
BMRB ID	:	17200
Title	:	NMR structure of UHRF1 Tandem Tudor Domains in a complex with Histone H3 peptide
Authors	:	Nady, N.; Lemak, A.; Fares, C.; Gutmanas, A.; Avvakumov, G.; Xue, S.; Arrowsmith, C.; Structural Genomics Consortium (SGC)
Deposited on	:	2010-09-21

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

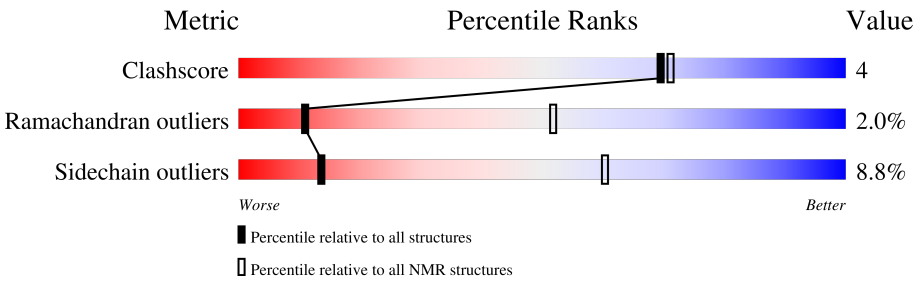
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 81%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	162	73% 14% • 10% •
2	B	11	64% 9% 27%

2 Ensemble composition and analysis (i)

This entry contains 15 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:127-A:163, A:177-A:283, B:2-B:8, B:10-B:10 (152)	0.81	12

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 2 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2785 atoms, of which 1372 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called E3 ubiquitin-protein ligase UHRF1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	161	2591	823	1268	235	259	6	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	GLY	-	expression tag	UNP Q96T88
A	125	GLY	-	expression tag	UNP Q96T88

- Molecule 2 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	11	194	53	104	20	17	0

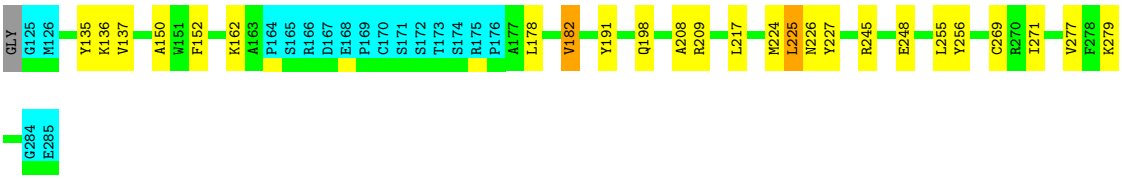
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

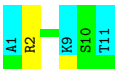
• Molecule 1: E3 ubiquitin-protein ligase UHRF1

Chain A: 73% 14% • 10% •



• Molecule 2: Histone H3

Chain B: 64% 9% 27%



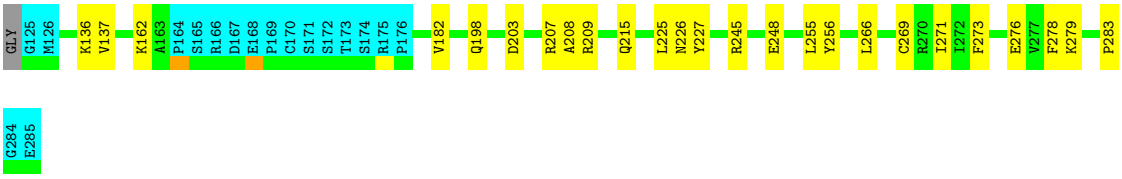
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: E3 ubiquitin-protein ligase UHRF1

Chain A: 73% 15% 10% •



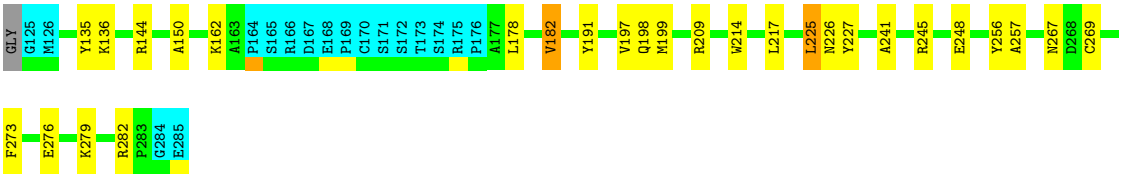
• Molecule 2: Histone H3

Chain B: 73% 27%

4.2.2 Score per residue for model 2

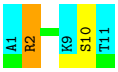
- Molecule 1: E3 ubiquitin-protein ligase UHRF1

Chain A: 72% 16% • 10% •



- Molecule 2: Histone H3

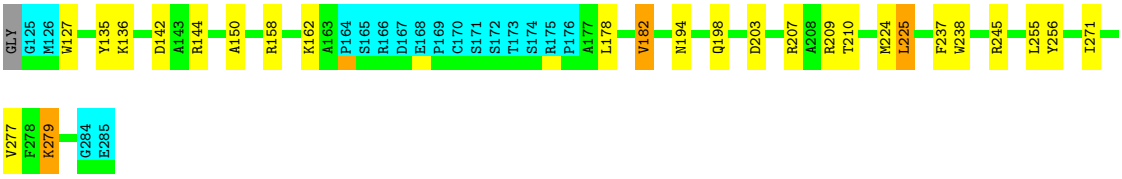
Chain B: 55% 9% 9% 27%



4.2.3 Score per residue for model 3

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

Chain A: 73% 14% • 10% •



- Molecule 2: Histone H3

Chain B: 73% 27%

4.2.4 Score per residue for model 4

- Molecule 1: E3 ubiquitin-protein ligase UHRF1

Chain A: 65% 20% • 10% •

GLY G125 M126 W127 D128 E129 T130 K136 V137 N138 D142 A143 R144 N147 A150 W151 F152 Q155 K162 A163 P164 S165 R166 D167 E168 P169 C170 S171 S172 T173 S174 R175 P176 A177 L178 V182 Y191 Q198 R202 A208 R209 T210 Q221 M224 L225 N226 Y227

W238 A241 R245 E248 L255 Y256 A257 N258 C269 R270 I271 I272 F273 K279 I280 E281 R282 P283 G284 E285

• Molecule 2: Histone H3

Chain B: 55% 18% 27%

A1 R2 K9 S10 T11

4.2.5 Score per residue for model 5

• Molecule 1: E3 ubiquitin-protein ligase UHRF1

Chain A: 69% 19% • 10% •

GLY G125 M126 E129 L132 K136 V137 N138 R144 A150 K162 A163 P164 S165 R166 D167 E168 P169 C170 S171 S172 T173 S174 R175 P176 V182 Y191 Q198 D203 A208 R209 T210 W214 L217 M224 L225 N226 R235 A241 E248 L255 Y256

A257 L266 N267 D268 C269 R270 I271 I272 F273 F278 K279 I280 P283 G284 E285

• Molecule 2: Histone H3

Chain B: 64% 9% 27%

A1 K4 K9 S10 T11

4.2.6 Score per residue for model 6

• Molecule 1: E3 ubiquitin-protein ligase UHRF1

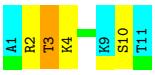
Chain A: 72% 15% • 10% •

GLY G125 M126 E129 K136 V137 N138 E139 Y140 R144 A150 W151 F152 K162 A163 P164 S165 R166 D167 E168 P169 C170 S171 S172 T173 S174 R175 P176 A177 L178 V182 Y188 Q198 D203 R207 A208 R209 M224 L225 F237 D240 E248 L255 N267

I271 E276 V277 F278 K279 I280 G284 E285

• Molecule 2: Histone H3

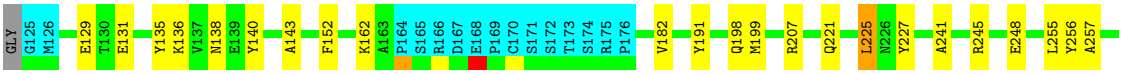
Chain B: 36% 27% 9% 27%

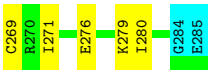


4.2.7 Score per residue for model 7

• Molecule 1: E3 ubiquitin-protein ligase UHRF1

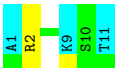
Chain A:





• Molecule 2: Histone H3

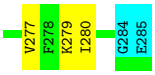
Chain B:



4.2.8 Score per residue for model 8

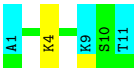
• Molecule 1: E3 ubiquitin-protein ligase UHRF1

Chain A:



• Molecule 2: Histone H3

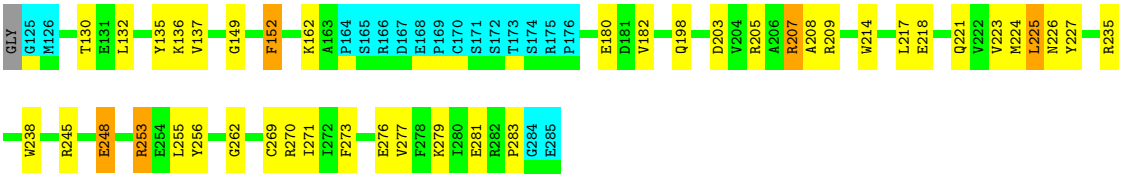
Chain B:



4.2.9 Score per residue for model 9

• Molecule 1: E3 ubiquitin-protein ligase UHRF1

Chain A:



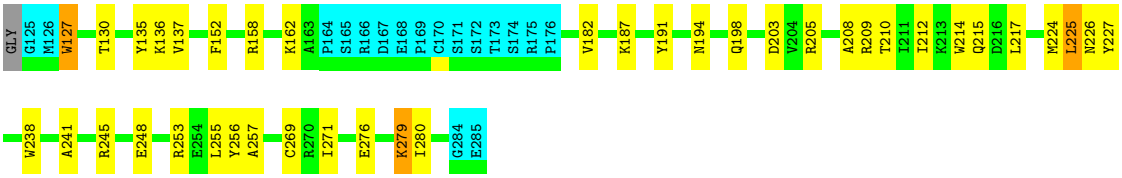
- Molecule 2: Histone H3

Chain B:

4.2.10 Score per residue for model 10

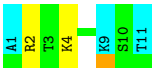
- Molecule 1: E3 ubiquitin-protein ligase UHRF1

Chain A:



- Molecule 2: Histone H3

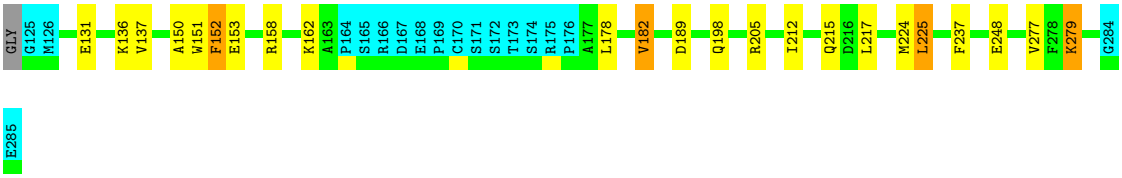
Chain B:



4.2.11 Score per residue for model 11

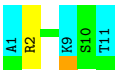
- Molecule 1: E3 ubiquitin-protein ligase UHRF1

Chain A:



- Molecule 2: Histone H3

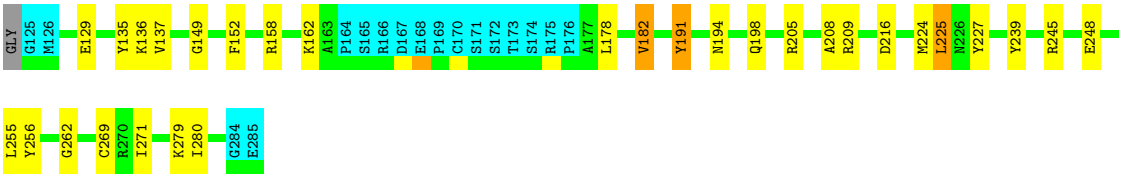
Chain B:



4.2.12 Score per residue for model 12 (medoid)

• Molecule 1: E3 ubiquitin-protein ligase UHRF1

Chain A:



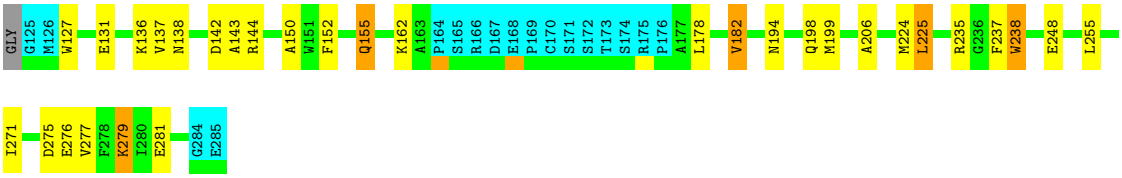
• Molecule 2: Histone H3

Chain B:

4.2.13 Score per residue for model 13

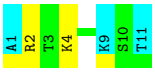
• Molecule 1: E3 ubiquitin-protein ligase UHRF1

Chain A:



• Molecule 2: Histone H3

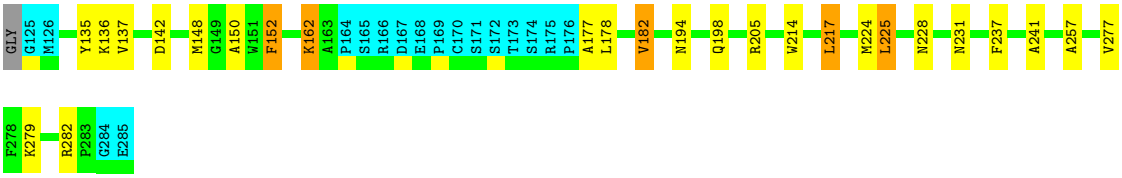
Chain B:



4.2.14 Score per residue for model 14

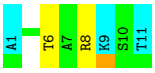
• Molecule 1: E3 ubiquitin-protein ligase UHRF1

Chain A:



• Molecule 2: Histone H3

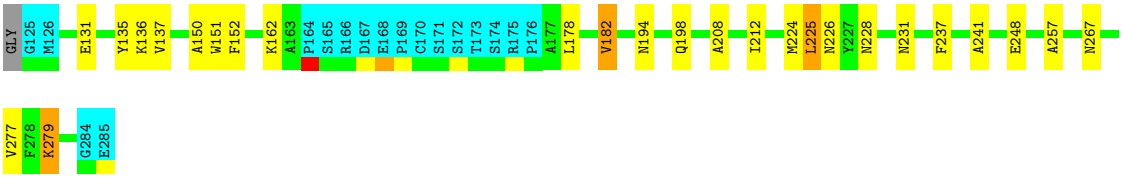
Chain B: 55% 18% 27%



4.2.15 Score per residue for model 15

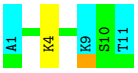
• Molecule 1: E3 ubiquitin-protein ligase UHRF1

Chain A: 73% 14% • 10% •



• Molecule 2: Histone H3

Chain B: 64% 9% 27%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	3.0
CNS	refinement	
TALOS	geometry optimization	

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1926
Number of shifts mapped to atoms	1926
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: M3L

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	0.87±0.01	0±0/1225 (0.0± 0.0%)	0.81±0.01	1±0/1663 (0.1± 0.0%)
2	B	0.87±0.07	0±0/64 (0.0± 0.0%)	0.77±0.07	0±0/83 (0.0± 0.0%)
All	All	0.87	0/19335 (0.0%)	0.81	19/26190 (0.1%)

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	225	LEU	N-CA-C	-6.46	93.57	111.00	15	15
1	A	225	LEU	CA-C-N	-5.42	105.29	117.20	6	4

There are no chirality outliers.

There are no planarity outliers.

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	1200	1158	1157	9±2
2	B	65	71	71	1±1
All	All	18975	18435	18420	140

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:ALA:HB1	1:A:237:PHE:HB2	0.69	1.65	3	6
1:A:142:ASP:HB2	1:A:207:ARG:HA	0.63	1.70	3	1
1:A:255:LEU:HB2	1:A:271:ILE:HB	0.62	1.68	12	10
1:A:224:MET:O	1:A:277:VAL:HA	0.60	1.97	15	6
1:A:226:ASN:HB3	1:A:273:PHE:HB2	0.59	1.74	9	5
1:A:214:TRP:HA	1:A:217:LEU:HD12	0.59	1.75	2	4
1:A:205:ARG:NH2	1:A:224:MET:SD	0.58	2.77	14	1
1:A:208:ALA:HB3	2:B:4:LYS:HE3	0.56	1.77	10	2
1:A:227:TYR:CZ	1:A:269:CYS:SG	0.56	2.99	2	2
1:A:143:ALA:HB1	1:A:199:MET:SD	0.54	2.42	13	2
1:A:138:ASN:HA	1:A:155:GLN:NE2	0.54	2.18	4	2
1:A:131:GLU:HA	1:A:280:ILE:HG21	0.53	1.79	7	2
1:A:227:TYR:CE1	1:A:269:CYS:SG	0.53	3.02	12	7
1:A:208:ALA:HB1	1:A:278:PHE:HB3	0.52	1.81	1	2
1:A:129:GLU:HB2	1:A:221:GLN:HG3	0.52	1.80	8	2
1:A:266:LEU:HB2	1:A:269:CYS:SG	0.52	2.45	5	1
1:A:208:ALA:HB2	1:A:224:MET:SD	0.51	2.45	9	2
1:A:276:GLU:HG2	2:B:2:ARG:HB3	0.50	1.82	2	1
1:A:147:ASN:HB2	2:B:10:SER:HB2	0.50	1.83	4	1
1:A:140:TYR:HB3	1:A:207:ARG:HD3	0.49	1.83	6	1
1:A:241:ALA:HB1	1:A:257:ALA:HB1	0.48	1.85	7	6
1:A:248:GLU:HA	1:A:253:ARG:HA	0.48	1.84	10	2
1:A:226:ASN:HB2	1:A:273:PHE:HB2	0.47	1.86	2	1
1:A:210:THR:HB	1:A:279:LYS:HD2	0.47	1.84	3	1
1:A:245:ARG:HB3	1:A:256:TYR:HB2	0.47	1.84	4	8
1:A:152:PHE:HB3	2:B:6:THR:HG21	0.47	1.87	14	1
2:B:3:THR:HG22	2:B:4:LYS:HG2	0.47	1.86	6	1
1:A:217:LEU:HD21	1:A:277:VAL:HG11	0.47	1.87	9	3
1:A:224:MET:SD	1:A:278:PHE:HB2	0.46	2.51	5	1
1:A:208:ALA:HB3	2:B:4:LYS:HD2	0.46	1.86	8	1
1:A:223:VAL:HG23	1:A:225:LEU:HD23	0.46	1.86	9	1
1:A:228:ASN:HB3	1:A:231:ASN:O	0.46	2.11	14	2
1:A:132:LEU:HB3	1:A:283:PRO:HD3	0.46	1.87	5	2
1:A:178:LEU:H	1:A:178:LEU:HD23	0.45	1.71	6	1
1:A:205:ARG:HD3	1:A:224:MET:SD	0.45	2.52	12	1
1:A:153:GLU:HG3	1:A:189:ASP:HB3	0.44	1.88	11	1
1:A:129:GLU:HG3	1:A:280:ILE:HG13	0.44	1.88	6	4
1:A:210:THR:HB	1:A:279:LYS:HE3	0.43	1.90	10	3
1:A:207:ARG:O	1:A:281:GLU:HG3	0.43	2.13	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:TYR:HB2	1:A:207:ARG:HD3	0.43	1.89	7	1
1:A:151:TRP:O	1:A:237:PHE:HB3	0.43	2.13	11	2
1:A:144:ARG:HA	1:A:150:ALA:O	0.43	2.14	5	6
1:A:212:ILE:HD11	1:A:279:LYS:HB3	0.43	1.91	15	2
1:A:178:LEU:O	1:A:182:VAL:HG13	0.43	2.14	14	8
1:A:130:THR:HG21	1:A:282:ARG:HG2	0.43	1.91	4	1
1:A:198:GLN:HE21	1:A:198:GLN:N	0.43	2.12	8	1
1:A:279:LYS:NZ	1:A:281:GLU:HA	0.43	2.29	13	1
1:A:148:MET:SD	1:A:237:PHE:CD1	0.43	3.11	14	1
1:A:276:GLU:HG2	2:B:2:ARG:HB2	0.42	1.90	6	1
1:A:226:ASN:HD22	1:A:276:GLU:HG3	0.42	1.73	10	2
1:A:225:LEU:HD23	1:A:239:TYR:O	0.42	2.15	12	1
1:A:218:GLU:HB2	1:A:221:GLN:HB2	0.41	1.92	9	1
1:A:238:TRP:CH2	2:B:4:LYS:HA	0.41	2.50	13	1
1:A:127:TRP:HZ3	1:A:212:ILE:HD12	0.41	1.75	10	1
1:A:276:GLU:HG2	2:B:2:ARG:N	0.41	2.30	7	1
1:A:197:VAL:HG12	1:A:199:MET:SD	0.41	2.56	2	1
1:A:149:GLY:HA3	1:A:262:GLY:N	0.41	2.31	12	2
1:A:205:ARG:HD2	1:A:224:MET:SD	0.41	2.56	10	1
1:A:205:ARG:HH22	1:A:208:ALA:HB2	0.41	1.74	12	1
1:A:241:ALA:HA	1:A:258:ASN:O	0.41	2.16	4	1
1:A:217:LEU:HD13	1:A:255:LEU:HG	0.40	1.93	5	1
1:A:127:TRP:HB3	1:A:221:GLN:NE2	0.40	2.31	4	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	144/162 (89%)	124±2 (86±1%)	17±2 (12±1%)	3±1 (2±1%)	11	53
2	B	8/11 (73%)	5±1 (67±16%)	2±1 (30±12%)	0±0 (3±6%)	6	37
All	All	2280/2595 (88%)	1937 (85%)	297 (13%)	46 (2%)	11	52

All 16 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	182	VAL	15
1	A	137	VAL	11
1	A	127	TRP	3
1	A	217	LEU	3
1	A	162	LYS	2
1	A	131	GLU	2
1	A	283	PRO	1
2	B	10	SER	1
2	B	3	THR	1
1	A	253	ARG	1
1	A	130	THR	1
1	A	280	ILE	1
1	A	206	ALA	1
2	B	2	ARG	1
1	A	177	ALA	1
2	B	8	ARG	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	128/143 (90%)	116±2 (91±2%)	12±2 (9±2%)	13	60
2	B	7/8 (88%)	7±0 (94±7%)	0±0 (6±7%)	24	73
All	All	2025/2265 (89%)	1846 (91%)	179 (9%)	13	60

All 41 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	136	LYS	15
1	A	162	LYS	15
1	A	198	GLN	15
1	A	279	LYS	15
1	A	248	GLU	12
1	A	225	LEU	11
1	A	135	TYR	9
1	A	209	ARG	8
1	A	152	PHE	7

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Mol	Chain	Res	Type	Models (Total)
1	A	203	ASP	6
1	A	194	ASN	6
1	A	238	TRP	5
1	A	215	GLN	4
1	A	267	ASN	4
2	B	2	ARG	4
1	A	158	ARG	4
1	A	191	TYR	3
1	A	142	ASP	3
1	A	138	ASN	3
1	A	235	ARG	3
1	A	205	ARG	3
1	A	207	ARG	2
1	A	266	LEU	2
1	A	276	GLU	2
1	A	214	TRP	2
1	A	128	ASP	1
1	A	202	ARG	1
2	B	4	LYS	1
1	A	178	LEU	1
1	A	224	MET	1
1	A	240	ASP	1
2	B	10	SER	1
1	A	213	LYS	1
1	A	237	PHE	1
1	A	180	GLU	1
1	A	270	ARG	1
1	A	187	LYS	1
1	A	216	ASP	1
1	A	131	GLU	1
1	A	155	GLN	1
1	A	226	ASN	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics

could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	M3L	B	9	2	10,11,12	1.22±0.10	1±1 (8±5%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	M3L	B	9	2	9,14,16	0.47±0.06	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	M3L	B	9	2	-	0±0,9,10,12	-

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	9	M3L	CB-CA	3.09	1.58	1.53	9	11
2	B	9	M3L	CE-NZ	2.09	1.57	1.51	14	1

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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	1926
Number of shifts mapped to atoms	1926
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	155	-0.24 ± 0.17	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	146	0.08 ± 0.22	None needed (< 0.5 ppm)
$^{13}C'$	141	0.09 ± 0.15	None needed (< 0.5 ppm)
^{15}N	145	-0.40 ± 0.51	None needed (< 0.5 ppm)

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 81%, i.e. 1766 atoms were assigned a chemical shift out of a possible 2174. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	689/758 (91%)	288/306 (94%)	268/304 (88%)	133/148 (90%)
Sidechain	971/1248 (78%)	675/798 (85%)	283/380 (74%)	13/70 (19%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	106/168 (63%)	66/80 (82%)	38/82 (46%)	2/6 (33%)
Overall	1766/2174 (81%)	1029/1184 (87%)	589/766 (77%)	148/224 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1917 atoms were assigned a chemical shift out of a possible 2387. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	758/849 (89%)	317/343 (92%)	296/342 (87%)	145/164 (88%)
Sidechain	1053/1370 (77%)	730/876 (83%)	310/418 (74%)	13/76 (17%)
Aromatic	106/168 (63%)	66/80 (82%)	38/82 (46%)	2/6 (33%)
Overall	1917/2387 (80%)	1113/1299 (86%)	644/842 (76%)	160/246 (65%)

7.1.4 Statistically unusual chemical shifts (i)

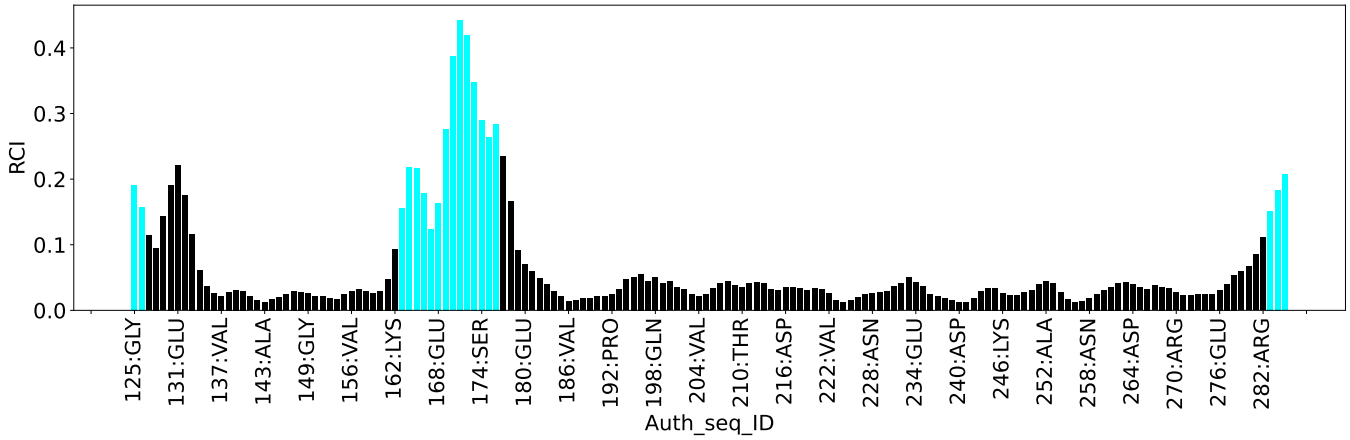
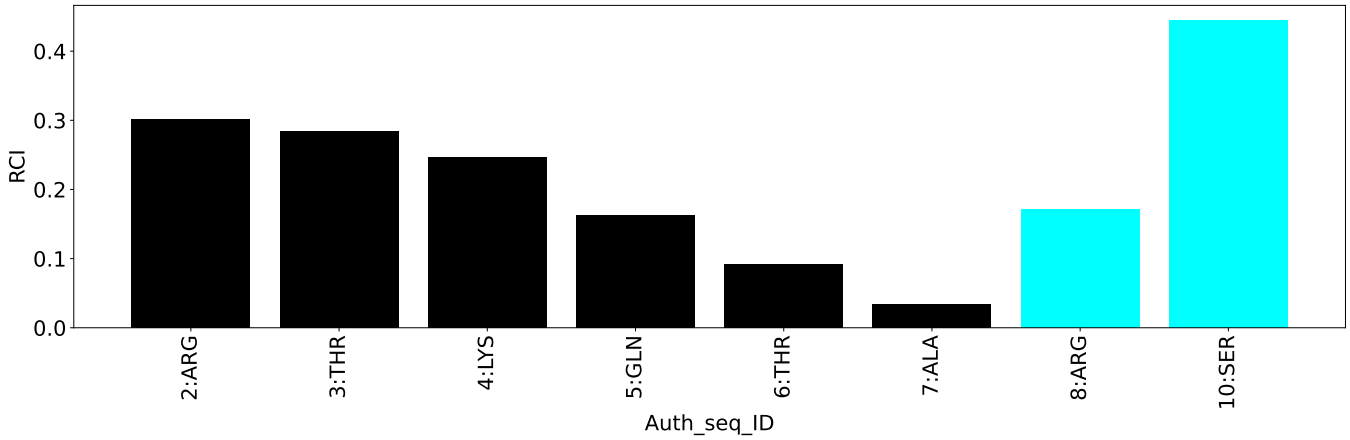
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	226	ASN	HB2	0.26	1.27 – 4.34	-8.3
1	A	226	ASN	HB3	0.26	1.12 – 4.38	-7.6
1	A	144	ARG	HG2	0.05	0.26 – 2.87	-5.8
1	A	144	ARG	HG3	0.00	0.15 – 2.94	-5.5

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B: