



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 10:46 PM BST

PDB ID : 2KDE
Title : NMR structure of major S5a (196-306):K48 linked diubiquitin species
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Deposited on : 2009-01-06

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

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

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

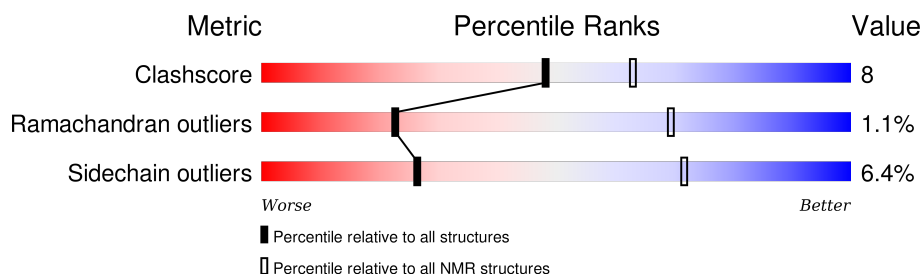
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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

Mol	Chain	Length	Quality of chain
1	A	111	
2	B	76	
2	C	76	

2 Ensemble composition and analysis

This entry contains 7 models. Model 3 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:206-A:295, B:1-B:76, C:77-C:150 (240)	2.13	3

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 1 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 6, 7
Single-model clusters	2; 5

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2027 atoms, of which 0 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					Trace
1	A	111	Total	C	N	O	S	0
			824	497	139	182	6	

- Molecule 2 is a protein called Ubiquitin.

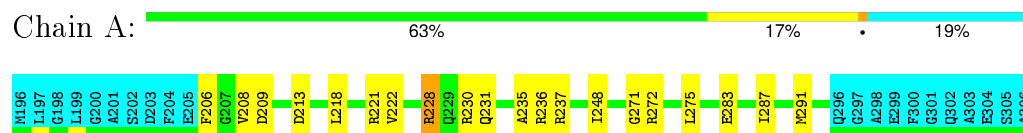
Mol	Chain	Residues	Atoms					Trace
2	B	76	Total	C	N	O	S	0
			601	378	105	117	1	
2	C	76	Total	C	N	O	S	0
			602	378	105	118	1	

4 Residue-property plots

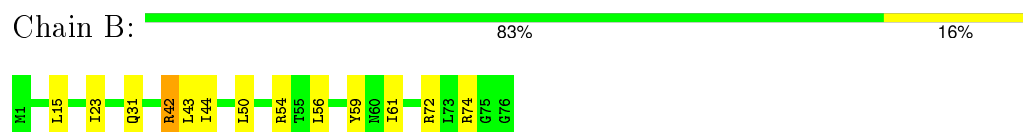
4.1 Average score per residue in the NMR ensemble

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.

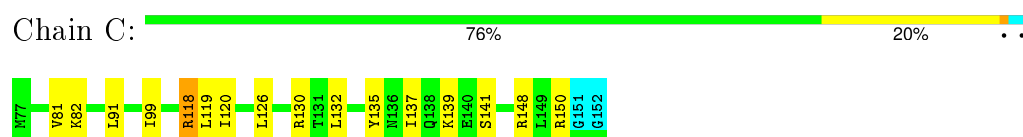
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4



- Molecule 2: Ubiquitin



- Molecule 2: Ubiquitin

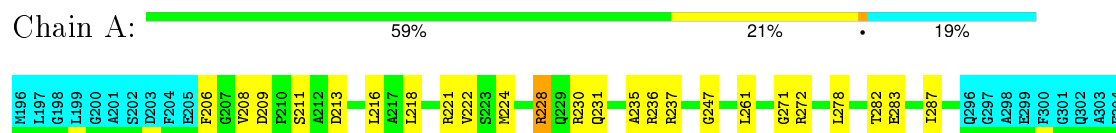


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1


- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4



S305
A306

- Molecule 2: Ubiquitin

Chain B:  74% 25%



- Molecule 2: Ubiquitin

Chain C:  72% 24%




4.2.2 Score per residue for model 2


- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A:  63% 16% 19%



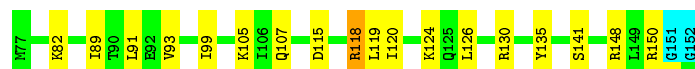
- Molecule 2: Ubiquitin

Chain B:  76% 22%



- Molecule 2: Ubiquitin

Chain C:  74% 22%



4.2.3 Score per residue for model 3 (medoid)


- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A:  57% 23% 19%




S305
A306

- Molecule 2: Ubiquitin

Chain B:  78% 18% ..

H1 L15 I23 I30 I36 R42 L43 L44 L50 L54 R54 T55 L56 Y59 R60 I61 S65 L71 R72 L73 R74 G75 G76

- Molecule 2: Ubiquitin

Chain C:  82% 14% ..

H77 R82 M101 R118 L119 L126 R130 T131 L132 Y135 M136 I137 Q138 K139 R148 R149 R150 G151 G152


4.2.4 Score per residue for model 4

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

Chain A:  64% 17% 19%

M196 L197 G198 L199 G200 A201 S202 D203 F204 E205 F206 G207 V208 D209 D213 L218 R221 V222 R228 Q229 R230 Q231 A235 R236 R237 D257 R272 L275 E283 I287 M291 Q296 G297 A298 E299 F300 G301 Q302 A303 E304 S305 A306

- Molecule 2: Ubiquitin

Chain B:  83% 16% .

H1 I13 T14 L15 Q31 R42 L43 I44 L50 R54 Y59 R63 R72 L73 R74 G75 G76

- Molecule 2: Ubiquitin

Chain C:  76% 20% ..

H77 V81 R82 L91 D108 R118 L119 I120 L126 R130 T131 L132 Y135 M136 I137 V146 R147 R148 L149 R150 G151 G152

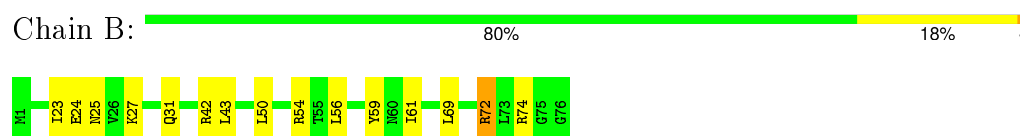
4.2.5 Score per residue for model 5

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4

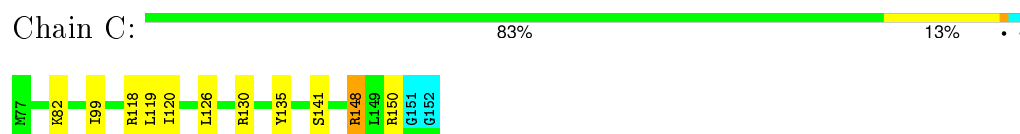
Chain A:  60% 19% . 19%

M196 L197 G198 L199 G200 A201 S202 D203 F204 E205 F206 L218 R221 V222 Q227 R228 Q229 R230 Q231 A235 R236 R237 A238 A239 A240 A241 S242 A243 A244 I248 D255 G271 R272 L278 I287 M291 Q296 G297 A298 E299 F300 G301 Q302 A303 E304 S305 A306

- Molecule 2: Ubiquitin



- Molecule 2: Ubiquitin

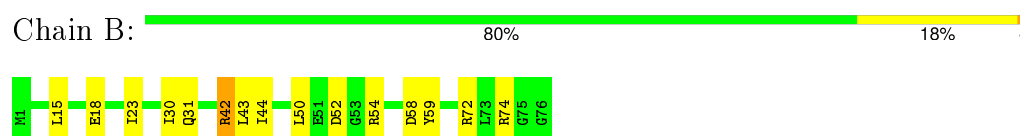


4.2.6 Score per residue for model 6

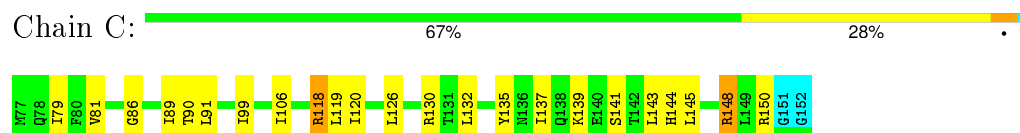
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4



- Molecule 2: Ubiquitin

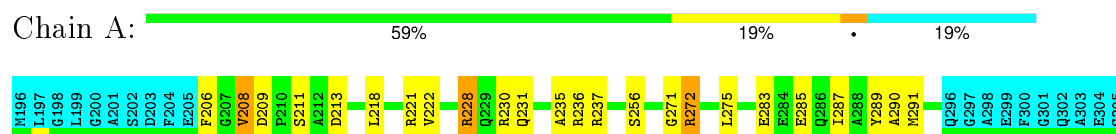


- Molecule 2: Ubiquitin



4.2.7 Score per residue for model 7

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 4



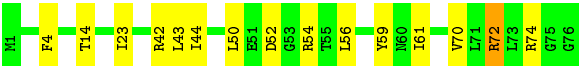
A306

● Molecule 2: Ubiquitin

Chain B:

80%

18%



● Molecule 2: Ubiquitin

Chain C:

71%

25%



5 Refinement protocol and experimental data overview ⓘ

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

Of the 30 calculated structures, 7 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
X-PLOR	structure solution	
X-PLOR	refinement	

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	6.0±0.0
2	B	0.0±0.0	4.0±0.0
2	C	0.0±0.0	4.0±0.0
All	All	0	98

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)
2	B	42	ARG	Sidechain	7
2	C	118	ARG	Sidechain	7
1	A	236	ARG	Sidechain	7
2	C	150	ARG	Sidechain	7
1	A	237	ARG	Sidechain	7
2	C	148	ARG	Sidechain	7
1	A	228	ARG	Sidechain	7
1	A	272	ARG	Sidechain	7
2	B	54	ARG	Sidechain	7
1	A	221	ARG	Sidechain	7
1	A	230	ARG	Sidechain	7
2	B	72	ARG	Sidechain	7
2	C	130	ARG	Sidechain	7
2	B	74	ARG	Sidechain	7

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	676	0	647	7±3
2	B	601	0	629	10±1
2	C	593	0	618	12±5
All	All	13090	0	13258	200

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:218:LEU:O	1:A:222:VAL:HG23	0.72	1.84	6	7
2:B:50:LEU:HD22	2:B:59:TYR:CG	0.70	2.21	3	6
2:C:119:LEU:C	2:C:120:ILE:HD12	0.69	2.08	5	3
2:C:81:VAL:HG21	2:C:91:LEU:HD22	0.68	1.63	1	3
2:B:23:ILE:HG22	2:B:27:LYS:CE	0.68	2.19	5	1
2:B:44:ILE:HD13	2:B:70:VAL:CG2	0.66	2.21	2	3
2:C:106:ILE:CD1	2:C:145:LEU:HD13	0.64	2.22	6	2
1:A:240:ALA:O	1:A:244:ALA:HB3	0.64	1.93	5	1
2:B:50:LEU:HD22	2:B:59:TYR:CD2	0.63	2.29	3	6
2:C:126:LEU:HD22	2:C:135:TYR:CD2	0.63	2.28	1	5
2:C:126:LEU:HD22	2:C:135:TYR:CG	0.62	2.29	2	7
2:B:23:ILE:HG23	2:B:43:LEU:HD12	0.62	1.71	2	5
2:B:43:LEU:HB3	2:B:50:LEU:HD12	0.61	1.71	5	2
1:A:283:GLU:O	1:A:287:ILE:HD12	0.61	1.96	2	6
2:B:23:ILE:HG22	2:B:27:LYS:HE3	0.61	1.72	5	1
2:C:119:LEU:HB3	2:C:126:LEU:HD12	0.60	1.72	1	3
2:C:99:ILE:HG23	2:C:119:LEU:HD12	0.60	1.72	1	4
2:B:44:ILE:HD13	2:B:70:VAL:HG23	0.58	1.73	2	2
2:B:44:ILE:HD12	2:B:44:ILE:N	0.58	2.14	2	3
2:B:44:ILE:N	2:B:44:ILE:HD12	0.58	2.14	3	3
2:C:120:ILE:HD12	2:C:120:ILE:N	0.57	2.15	2	1
2:C:120:ILE:N	2:C:120:ILE:HD12	0.57	2.14	4	2
1:A:290:ALA:HB1	2:C:144:HIS:HB3	0.56	1.75	7	1
2:C:90:THR:C	2:C:91:LEU:HD12	0.55	2.22	6	1
1:A:215:GLU:OE1	2:B:73:LEU:HD11	0.55	2.01	3	1
2:C:106:ILE:HD13	2:C:145:LEU:HD13	0.55	1.78	6	1
2:C:132:LEU:HA	2:C:137:ILE:HD12	0.55	1.78	6	4
1:A:210:PRO:CB	1:A:217:ALA:HB2	0.54	2.32	6	2
2:B:73:LEU:HD12	2:B:73:LEU:N	0.54	2.18	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:15:LEU:HD11	2:B:30:ILE:HG12	0.53	1.79	6	3
2:B:43:LEU:CD1	2:B:69:LEU:HD12	0.53	2.34	5	1
1:A:206:PHE:O	1:A:216:LEU:HD13	0.53	2.03	6	1
2:B:4:PHE:CZ	2:B:14:THR:HG23	0.52	2.40	1	1
1:A:248:ILE:O	1:A:248:ILE:HG23	0.52	2.05	3	3
1:A:239:ALA:O	1:A:243:ALA:HB3	0.52	2.04	5	1
1:A:287:ILE:HG23	1:A:291:MET:CE	0.52	2.35	7	3
1:A:253:THR:O	1:A:253:THR:HG23	0.51	2.06	2	2
2:B:42:ARG:HB3	2:B:44:ILE:HD11	0.51	1.83	1	4
2:B:56:LEU:HA	2:B:61:ILE:HD12	0.50	1.83	3	4
1:A:278:LEU:HD22	2:C:84:LEU:HD13	0.50	1.82	1	1
2:C:89:ILE:HG22	2:C:91:LEU:CD1	0.50	2.36	6	1
1:A:287:ILE:HG23	1:A:291:MET:HE3	0.49	1.84	4	1
1:A:210:PRO:HB2	1:A:217:ALA:HB2	0.49	1.82	6	1
2:C:91:LEU:HD12	2:C:91:LEU:N	0.49	2.23	1	1
2:C:89:ILE:HG22	2:C:91:LEU:CD2	0.49	2.37	2	1
2:B:4:PHE:CE1	2:B:14:THR:HG23	0.48	2.42	7	1
2:C:81:VAL:HG11	2:C:106:ILE:HD11	0.48	1.84	6	1
2:C:91:LEU:N	2:C:91:LEU:HD12	0.48	2.24	6	1
2:C:99:ILE:CG2	2:C:119:LEU:HD12	0.48	2.38	1	4
1:A:231:GLN:O	1:A:235:ALA:HB2	0.47	2.08	3	6
1:A:287:ILE:HG23	1:A:291:MET:HE2	0.47	1.86	7	1
2:C:93:VAL:HG12	2:C:105:LYS:CD	0.47	2.40	2	1
2:B:23:ILE:HG22	2:B:27:LYS:HE2	0.46	1.86	5	1
2:C:99:ILE:HG23	2:C:119:LEU:CD1	0.46	2.40	1	2
2:C:126:LEU:CD2	2:C:135:TYR:CD1	0.45	3.00	3	5
2:C:89:ILE:HG22	2:C:91:LEU:HD12	0.45	1.86	7	1
2:B:23:ILE:CG2	2:B:43:LEU:HD12	0.45	2.41	2	2
2:C:126:LEU:CD2	2:C:135:TYR:CG	0.45	2.99	1	5
1:A:243:ALA:HB1	1:A:249:ALA:HB2	0.45	1.89	6	1
2:C:94:GLU:O	2:C:132:LEU:HD12	0.44	2.12	1	1
2:B:6:LYS:HG2	2:B:12:THR:HG23	0.44	1.89	2	1
2:C:91:LEU:HD21	2:C:106:ILE:CG1	0.44	2.41	1	2
2:B:43:LEU:C	2:B:44:ILE:HD12	0.44	2.33	4	3
1:A:294:SER:CB	2:C:144:HIS:CE1	0.44	3.00	6	1
2:B:4:PHE:CE1	2:B:14:THR:CG2	0.44	3.00	7	1
2:B:50:LEU:CD2	2:B:59:TYR:CD1	0.44	3.00	7	2
2:B:43:LEU:HD12	2:B:69:LEU:HD12	0.44	1.90	5	1
2:B:50:LEU:CD2	2:B:59:TYR:CG	0.44	3.00	5	2
2:C:79:ILE:HD12	2:C:143:LEU:HD12	0.44	1.90	6	1
2:B:73:LEU:N	2:B:73:LEU:HD12	0.44	2.27	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:81:VAL:CG2	2:C:91:LEU:HD12	0.44	2.43	4	1
1:A:275:LEU:HD11	1:A:277:ASP:OD2	0.44	2.13	6	1
1:A:291:MET:HE2	2:C:124:LYS:N	0.43	2.28	2	1
2:B:18:GLU:O	2:B:56:LEU:HD12	0.43	2.14	2	1
2:C:81:VAL:HG11	2:C:106:ILE:CD1	0.43	2.44	6	1
2:B:36:ILE:HG21	2:B:71:LEU:HD21	0.43	1.89	3	1
2:C:89:ILE:CG2	2:C:91:LEU:HD11	0.43	2.44	6	1
2:C:126:LEU:HD22	2:C:135:TYR:CD1	0.43	2.49	4	1
1:A:261:LEU:C	1:A:261:LEU:HD23	0.43	2.34	3	1
1:A:213:ASP:OD2	1:A:216:LEU:HD13	0.42	2.14	1	1
2:B:15:LEU:HD11	2:B:30:ILE:CG1	0.42	2.44	6	1
1:A:208:VAL:HG23	1:A:209:ASP:N	0.42	2.30	4	2
2:C:126:LEU:CD2	2:C:135:TYR:CD2	0.42	3.02	4	1
1:A:208:VAL:HG13	1:A:209:ASP:N	0.42	2.30	7	3
2:B:44:ILE:CD1	2:B:44:ILE:N	0.42	2.83	1	1
1:A:275:LEU:HD11	1:A:277:ASP:CG	0.41	2.35	6	1
2:B:44:ILE:N	2:B:44:ILE:CD1	0.41	2.83	2	3
2:C:120:ILE:N	2:C:120:ILE:CD1	0.41	2.83	4	2
2:B:50:LEU:CD2	2:B:59:TYR:CD2	0.41	3.03	4	1
2:B:43:LEU:HD12	2:B:43:LEU:N	0.41	2.30	5	1
2:C:99:ILE:HG22	2:C:103:LYS:HE3	0.41	1.92	1	1
1:A:291:MET:HE2	2:C:120:ILE:HG23	0.41	1.93	6	1
2:C:146:VAL:HG12	2:C:147:LEU:N	0.41	2.30	4	1
2:C:91:LEU:CD1	2:C:91:LEU:N	0.40	2.84	6	2
2:C:118:ARG:HB3	2:C:120:ILE:HD11	0.40	1.92	4	1
2:B:13:ILE:HG22	2:B:15:LEU:CD2	0.40	2.46	4	1
2:C:91:LEU:HD23	2:C:102:VAL:HG13	0.40	1.92	7	1
2:B:45:PHE:HB2	2:B:67:LEU:HD23	0.40	1.93	2	1
1:A:248:ILE:HG23	1:A:249:ALA:N	0.40	2.31	2	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	90/111 (81%)	78±2 (87±2%)	9±2 (10±3%)	2±1 (3±1%)	11	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	74/76 (97%)	69±2 (93±3%)	5±2 (7±3%)	0±0 (0±0%)	56 85
2	C	73/76 (96%)	68±1 (94±1%)	4±1 (6±1%)	0±0 (0±0%)	56 85
All	All	1659/1841 (90%)	1510 (91%)	131 (8%)	18 (1%)	23 69

All 8 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	206	PHE	6
1	A	271	GLY	5
1	A	282	THR	2
1	A	247	GLY	1
2	C	86	GLY	1
2	B	75	GLY	1
1	A	208	VAL	1
1	A	252	GLY	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	70/83 (84%)	64±2 (91±3%)	6±2 (9±3%)	17 62
2	B	68/68 (100%)	65±1 (95±1%)	3±1 (5±1%)	38 81
2	C	68/68 (100%)	64±1 (94±2%)	4±1 (6±2%)	29 74
All	All	1442/1533 (94%)	1349 (94%)	93 (6%)	26 72

All 49 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	228	ARG	6
1	A	275	LEU	5
2	C	141	SER	5
2	C	139	LYS	4
2	B	31	GLN	4

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Mol	Chain	Res	Type	Models (Total)
2	C	82	LYS	4
1	A	213	ASP	4
2	C	148	ARG	3
2	B	72	ARG	3
2	C	118	ARG	3
2	B	52	ASP	2
1	A	242	SER	2
1	A	256	SER	2
2	B	65	SER	2
1	A	221	ARG	2
1	A	272	ARG	2
1	A	227	GLN	2
2	C	107	GLN	2
1	A	211	SER	2
2	B	42	ARG	2
1	A	285	GLU	2
2	B	63	LYS	2
1	A	220	LEU	2
1	A	278	LEU	1
2	B	62	GLN	1
2	B	18	GLU	1
2	B	74	ARG	1
2	C	101	ASN	1
1	A	257	ASP	1
1	A	229	GLN	1
1	A	279	SER	1
2	B	58	ASP	1
2	C	108	ASP	1
1	A	289	TYR	1
1	A	226	GLU	1
1	A	237	ARG	1
1	A	224	MET	1
1	A	255	ASP	1
2	C	130	ARG	1
1	A	261	LEU	1
2	B	24	GLU	1
2	C	115	ASP	1
2	C	78	GLN	1
2	B	25	ASN	1
2	C	127	GLU	1
1	A	216	LEU	1
1	A	209	ASP	1

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Mol	Chain	Res	Type	Models (Total)
2	C	143	LEU	1
2	B	32	ASP	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