



Full wwPDB NMR Structure Validation Report ⓘ

Feb 20, 2018 – 03:31 am GMT

PDB ID : 2K07
Title : Solution NMR structure of human E2-like ubiquitin-fold modifier conjugating enzyme 1 (UFC1). Northeast Structural Genomics Consortium target HR41
Authors : Liu, G.; Eletsky, A.; Atreya, H.S.; Aramini, J.M.; Xiao, R.; Acton, T.; Montelione, G.T.; Szyperski, T.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2008-01-25

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 ⓘ 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
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk30686
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30686

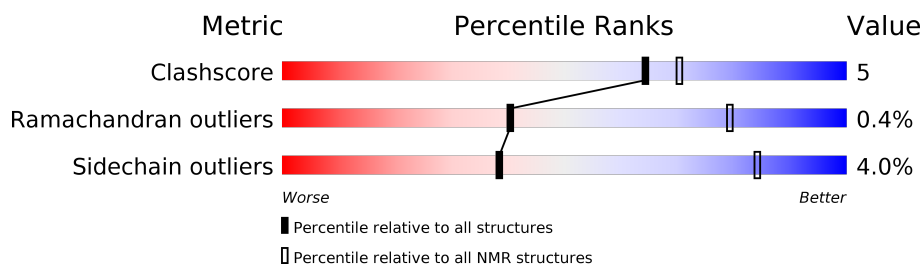
1 Overall quality at a glance

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	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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	175	

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 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:5-A:106, A:113-A:159 (149)	0.65	15

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 4 clusters and 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2888 atoms, of which 1437 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ufm1-conjugating enzyme 1.

Mol	Chain	Residues	Atoms						Trace
1	A	175	Total	C	H	N	O	S	0
			2888	931	1437	258	256	6	

There are 8 discrepancies between the modelled and reference sequences:

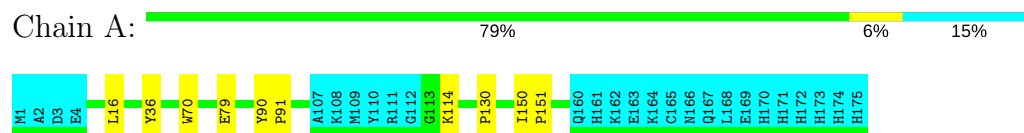
Chain	Residue	Modelled	Actual	Comment	Reference
A	168	LEU	-	EXPRESSION TAG	UNP Q9Y3C8
A	169	GLU	-	EXPRESSION TAG	UNP Q9Y3C8
A	170	HIS	-	EXPRESSION TAG	UNP Q9Y3C8
A	171	HIS	-	EXPRESSION TAG	UNP Q9Y3C8
A	172	HIS	-	EXPRESSION TAG	UNP Q9Y3C8
A	173	HIS	-	EXPRESSION TAG	UNP Q9Y3C8
A	174	HIS	-	EXPRESSION TAG	UNP Q9Y3C8
A	175	HIS	-	EXPRESSION TAG	UNP Q9Y3C8

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: Ufm1-conjugating enzyme 1

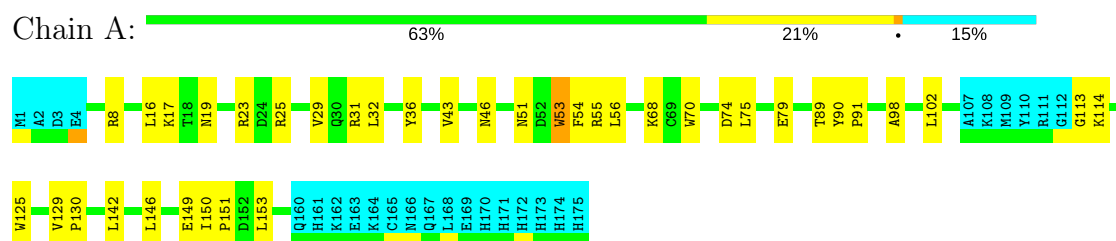


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

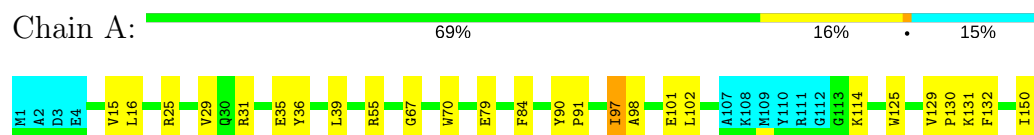
4.2.1 Score per residue for model 1

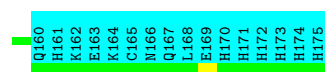
- Molecule 1: Ufm1-conjugating enzyme 1



4.2.2 Score per residue for model 2

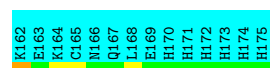
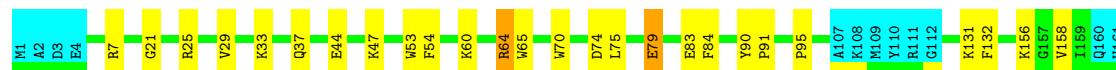
- Molecule 1: Ufm1-conjugating enzyme 1





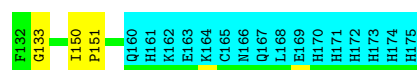
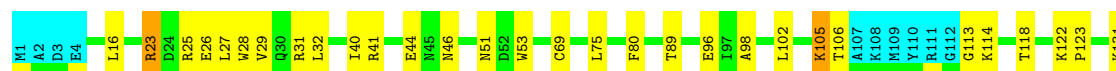
4.2.3 Score per residue for model 3

- Molecule 1: Ufm1-conjugating enzyme 1



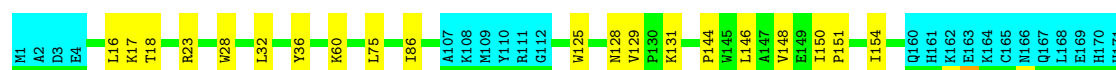
4.2.4 Score per residue for model 4

- Molecule 1: Ufm1-conjugating enzyme 1



4.2.5 Score per residue for model 5

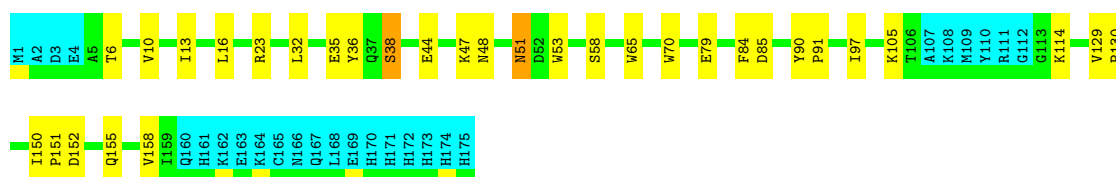
- Molecule 1: Ufm1-conjugating enzyme 1



4.2.6 Score per residue for model 6

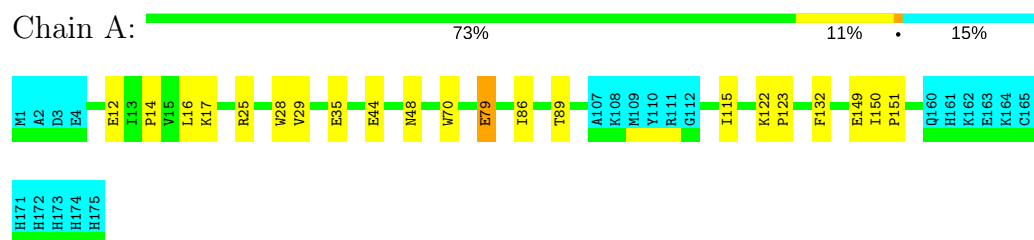
- Molecule 1: Ufm1-conjugating enzyme 1





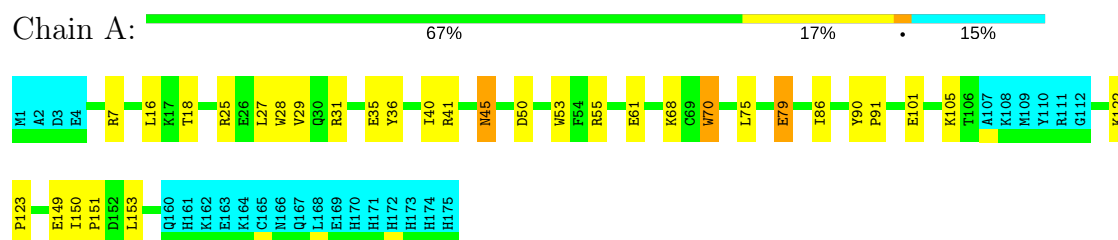
4.2.7 Score per residue for model 7

- Molecule 1: Ufm1-conjugating enzyme 1



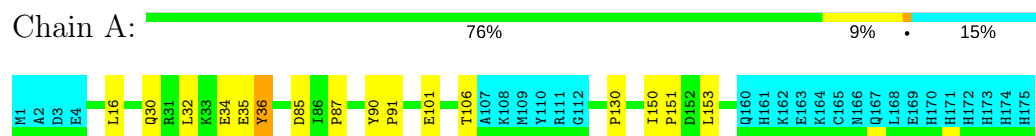
4.2.8 Score per residue for model 8

- Molecule 1: Ufm1-conjugating enzyme 1



4.2.9 Score per residue for model 9

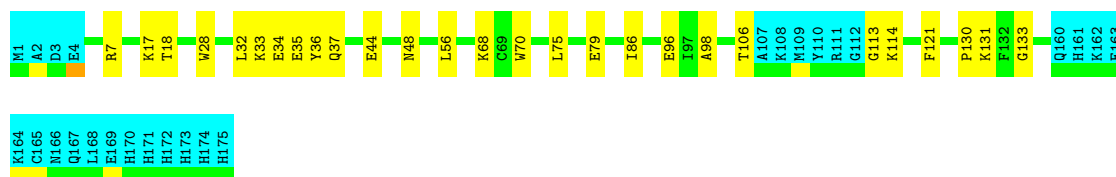
- Molecule 1: Ufm1-conjugating enzyme 1



4.2.10 Score per residue for model 10

- Molecule 1: Ufm1-conjugating enzyme 1





4.2.11 Score per residue for model 11

- Molecule 1: Ufm1-conjugating enzyme 1

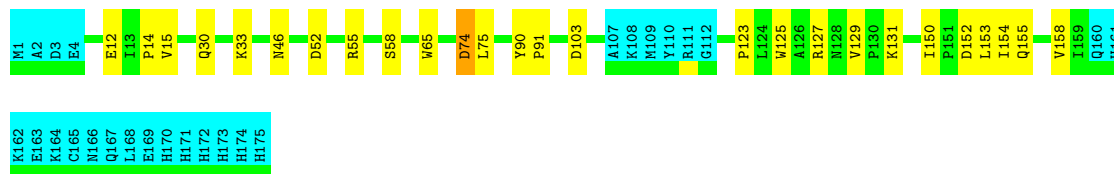
Chain A: 75% 9% 15%



4.2.12 Score per residue for model 12

- Molecule 1: Ufm1-conjugating enzyme 1

Chain A: 70% 14% 15%



4.2.13 Score per residue for model 13

- Molecule 1: Ufm1-conjugating enzyme 1

Chain A: 75% 10% 15%



4.2.14 Score per residue for model 14

- Molecule 1: Ufm1-conjugating enzyme 1

Chain A: 71% 14% 15%



Y166
Q167
L168
E169
H170
H171
H172
H173
H174
H175

4.2.15 Score per residue for model 15 (medoid)


- Molecule 1: Ufm1-conjugating enzyme 1

Chain A: 

M1 A2 D3 E4 R25 E26 L27 V29 L32 Y36 L39 L40 R41 Y42 V43 E79 E96 A107 K108 M109 Y110 R111 G112 G113 K114 M125 L137 I150 I154 Q160 H161 K162 E163 K164 C165 N166 Q167 L168 E169 H170 H171 H172 H173 H174 H175

4.2.16 Score per residue for model 16

- Molecule 1: Ufm1-conjugating enzyme 1

Chain A: 

M1 A2 D3 E4 T6 P14 S38 V43 R47 D85 I86 P87 Y90 P91 E96 A107 K108 M109 Y110 R111 G112 G113 K114 V129 P130 L142 L146 P151 D152 L153 Q160 H161 K162 E163 C164 C165 N166 Q167 L168 E169 H170 H171 H172 H173 H174 H175

4.2.17 Score per residue for model 17

- Molecule 1: Ufm1-conjugating enzyme 1

Chain A: 

M1 A2 D3 E4 L16 N19 R23 V28 R31 L32 E35 Y36 R41 R55 E83 I86 Y90 P91 D103 A107 K108 M109 Y110 R111 G112 G113 K114 L117 T118 F121 K122 P123 N128 V129 P130 F132 G141 L153 K156 G157

Y168
Y169
Q160
H161
K162
E163
K164
C165
N166
Q167
L168
E169
H170
H171
H172
H173
H174
H175

4.2.18 Score per residue for model 18

- Molecule 1: Ufm1-conjugating enzyme 1

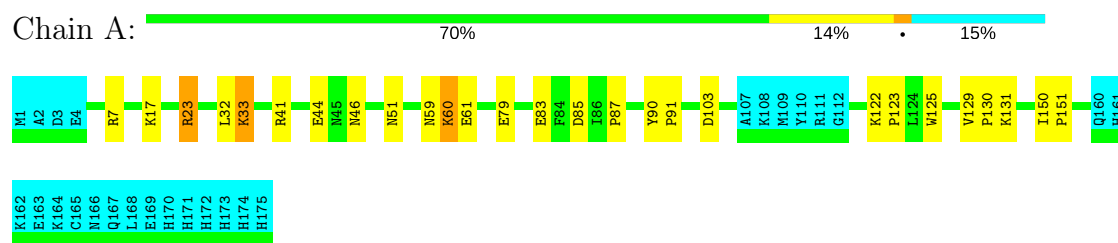
Chain A: 

M1 A2 D3 E4 E7 R23 R31 E35 L39 L40 R41 N46 N61 W70 D74 Y78 E79 F84 T89 T97 A107 K108 M109 Y110 R111 G112 G113 L134 A135 I150 P151 Q160 H161 K162 E163 K164 C165 N166 Q167 L168 E169 H170 H171

H172
H173
H174
H175

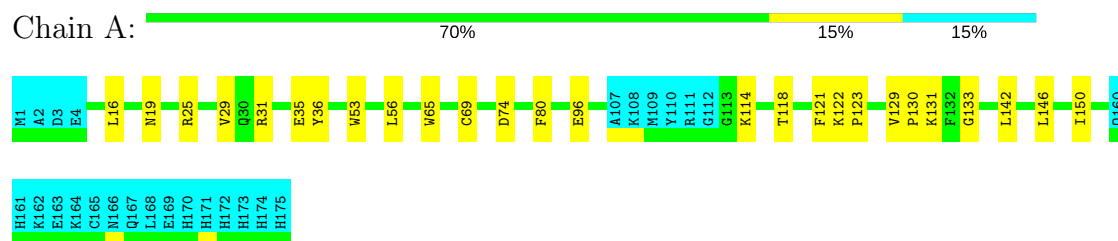
4.2.19 Score per residue for model 19

- Molecule 1: Ufm1-conjugating enzyme 1



4.2.20 Score per residue for model 20

- Molecule 1: Ufm1-conjugating enzyme 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics, simulated annealing, distance geometry, torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CNS	refinement	1.1
CYANA	refinement	2.1
CYANA	structure solution	2.1

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.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [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	1225	1227	1224	11±4
All	All	24500	24540	24480	226

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:GLU:HB2	1:A:114:LYS:HD3	0.81	1.51	15	2
1:A:65:TRP:HB2	1:A:84:PHE:HB2	0.80	1.53	3	2
1:A:16:LEU:HD21	1:A:35:GLU:HB3	0.78	1.54	14	5
1:A:102:LEU:HA	1:A:105:LYS:HD3	0.66	1.67	4	1
1:A:16:LEU:O	1:A:131:LYS:HA	0.64	1.92	5	2
1:A:23:ARG:HA	1:A:23:ARG:HE	0.62	1.54	19	2
1:A:96:GLU:HB3	1:A:114:LYS:HD3	0.61	1.71	20	1
1:A:90:TYR:CD1	1:A:91:PRO:HA	0.61	2.31	3	10
1:A:16:LEU:HD21	1:A:35:GLU:HG2	0.59	1.74	2	1
1:A:68:LYS:HD3	1:A:70:TRP:CZ3	0.59	2.33	8	1
1:A:70:TRP:CD1	1:A:79:GLU:HB3	0.58	2.34	10	4
1:A:105:LYS:HG2	1:A:158:VAL:HG11	0.58	1.74	6	1
1:A:70:TRP:HB3	1:A:79:GLU:HA	0.57	1.75	13	2
1:A:102:LEU:HD22	1:A:153:LEU:HG	0.57	1.74	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:ARG:NH2	1:A:91:PRO:HG3	0.57	2.14	14	1
1:A:33:LYS:O	1:A:37:GLN:HG2	0.57	2.00	13	3
1:A:16:LEU:HD21	1:A:35:GLU:HB2	0.57	1.76	8	2
1:A:96:GLU:HB3	1:A:114:LYS:HD2	0.56	1.78	14	1
1:A:96:GLU:CB	1:A:114:LYS:HD2	0.55	2.32	14	2
1:A:46:ASN:ND2	1:A:52:ASP:HA	0.55	2.17	14	2
1:A:69:CYS:SG	1:A:80:PHE:HB2	0.55	2.42	20	2
1:A:46:ASN:HB3	1:A:51:ASN:O	0.54	2.02	1	4
1:A:98:ALA:HA	1:A:113:GLY:HA3	0.54	1.78	10	1
1:A:70:TRP:HB3	1:A:79:GLU:HB3	0.54	1.78	7	2
1:A:89:THR:HG22	1:A:92:THR:HB	0.53	1.80	14	1
1:A:150:ILE:N	1:A:151:PRO:HD2	0.53	2.18	1	8
1:A:98:ALA:HB2	1:A:114:LYS:HG2	0.53	1.78	2	1
1:A:55:ARG:HA	1:A:55:ARG:NE	0.53	2.19	1	1
1:A:53:TRP:HB3	1:A:54:PHE:HD1	0.53	1.62	1	1
1:A:16:LEU:HD23	1:A:31:ARG:HG3	0.53	1.80	17	1
1:A:146:LEU:O	1:A:150:ILE:HB	0.52	2.05	20	3
1:A:60:LYS:HA	1:A:60:LYS:HE3	0.52	1.81	19	1
1:A:64:ARG:HH22	1:A:83:GLU:HB3	0.51	1.64	3	1
1:A:43:VAL:O	1:A:47:LYS:HG2	0.51	2.06	16	1
1:A:32:LEU:O	1:A:36:TYR:HB2	0.50	2.06	9	2
1:A:43:VAL:HG21	1:A:55:ARG:HH21	0.50	1.67	1	1
1:A:152:ASP:O	1:A:155:GLN:HG3	0.49	2.07	12	1
1:A:142:LEU:O	1:A:146:LEU:HG	0.49	2.07	16	3
1:A:31:ARG:NH2	1:A:133:GLY:HA2	0.49	2.22	20	3
1:A:84:PHE:CZ	1:A:97:ILE:HG12	0.49	2.43	6	1
1:A:25:ARG:O	1:A:29:VAL:HG23	0.49	2.07	15	8
1:A:30:GLN:HG3	1:A:33:LYS:HE3	0.49	1.83	13	1
1:A:39:LEU:HD23	1:A:135:ALA:HB2	0.49	1.85	18	1
1:A:152:ASP:HA	1:A:155:GLN:HG2	0.48	1.84	6	1
1:A:68:LYS:HD3	1:A:70:TRP:HZ3	0.48	1.69	8	1
1:A:28:TRP:CH2	1:A:86:ILE:HG21	0.48	2.43	7	6
1:A:12:GLU:O	1:A:14:PRO:HD3	0.48	2.09	7	2
1:A:158:VAL:HG23	1:A:159:ILE:HG13	0.48	1.85	17	1
1:A:122:LYS:HB2	1:A:123:PRO:HD3	0.47	1.87	8	3
1:A:35:GLU:O	1:A:39:LEU:HG	0.47	2.10	18	2
1:A:129:VAL:HG13	1:A:130:PRO:HA	0.47	1.86	16	3
1:A:102:LEU:O	1:A:106:THR:HG22	0.47	2.09	4	1
1:A:90:TYR:CG	1:A:91:PRO:HA	0.47	2.44	1	4
1:A:98:ALA:HA	1:A:113:GLY:O	0.47	2.09	1	2
1:A:30:GLN:O	1:A:34:GLU:HG2	0.46	2.10	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ARG:HE	1:A:23:ARG:HA	0.46	1.69	17	1
1:A:125:TRP:O	1:A:129:VAL:HG23	0.46	2.11	5	6
1:A:16:LEU:HD23	1:A:31:ARG:HG2	0.46	1.86	1	1
1:A:17:LYS:HD2	1:A:17:LYS:N	0.46	2.26	19	1
1:A:96:GLU:HB3	1:A:114:LYS:HA	0.46	1.87	10	1
1:A:131:LYS:HB2	1:A:131:LYS:NZ	0.46	2.26	3	1
1:A:35:GLU:HA	1:A:38:SER:OG	0.46	2.11	6	1
1:A:60:LYS:H	1:A:60:LYS:HD3	0.45	1.72	3	1
1:A:15:VAL:HB	1:A:131:LYS:O	0.45	2.11	12	1
1:A:25:ARG:HA	1:A:28:TRP:HB3	0.45	1.88	4	1
1:A:144:PRO:O	1:A:148:VAL:HG23	0.45	2.11	5	1
1:A:85:ASP:O	1:A:87:PRO:HD3	0.45	2.12	9	4
1:A:23:ARG:NE	1:A:23:ARG:HA	0.45	2.26	1	3
1:A:53:TRP:HB3	1:A:54:PHE:CD2	0.45	2.47	3	1
1:A:36:TYR:O	1:A:40:ILE:HG13	0.45	2.11	14	2
1:A:75:LEU:HD13	1:A:75:LEU:O	0.45	2.10	3	1
1:A:150:ILE:O	1:A:154:ILE:HG13	0.45	2.12	12	4
1:A:96:GLU:CB	1:A:114:LYS:HD3	0.45	2.42	16	1
1:A:84:PHE:HB3	1:A:97:ILE:HA	0.45	1.88	11	3
1:A:118:THR:OG1	1:A:121:PHE:HB2	0.45	2.12	17	1
1:A:21:GLY:HA3	1:A:90:TYR:O	0.44	2.12	3	1
1:A:153:LEU:HG	1:A:158:VAL:HB	0.44	1.89	12	1
1:A:35:GLU:OE1	1:A:133:GLY:HA3	0.44	2.12	10	1
1:A:53:TRP:HA	1:A:70:TRP:CD1	0.44	2.48	8	1
1:A:153:LEU:HA	1:A:156:LYS:HE2	0.44	1.88	2	1
1:A:156:LYS:HE3	1:A:158:VAL:HG21	0.44	1.89	3	1
1:A:19:ASN:HA	1:A:31:ARG:HD3	0.44	1.89	17	1
1:A:106:THR:HG23	1:A:153:LEU:HD11	0.44	1.90	9	1
1:A:150:ILE:HB	1:A:151:PRO:HD3	0.44	1.87	8	3
1:A:56:LEU:HD21	1:A:65:TRP:HB3	0.44	1.88	20	1
1:A:23:ARG:HA	1:A:23:ARG:NE	0.44	2.25	4	1
1:A:17:LYS:HG2	1:A:34:GLU:OE1	0.44	2.12	14	1
1:A:30:GLN:O	1:A:33:LYS:HG2	0.43	2.13	12	1
1:A:123:PRO:O	1:A:127:ARG:HG3	0.43	2.13	12	1
1:A:28:TRP:O	1:A:32:LEU:HG	0.43	2.13	4	1
1:A:44:GLU:OE2	1:A:47:LYS:HD3	0.43	2.13	6	1
1:A:33:LYS:HB3	1:A:33:LYS:NZ	0.43	2.28	19	1
1:A:90:TYR:CE1	1:A:95:PRO:HD3	0.43	2.49	3	1
1:A:130:PRO:O	1:A:131:LYS:HB2	0.43	2.13	20	4
1:A:14:PRO:HD2	1:A:38:SER:HA	0.43	1.91	16	1
1:A:70:TRP:HA	1:A:78:TYR:O	0.43	2.14	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:ARG:O	1:A:67:GLY:HA3	0.43	2.14	2	1
1:A:105:LYS:NZ	1:A:105:LYS:HB2	0.43	2.28	8	1
1:A:13:ILE:HG23	1:A:38:SER:HB2	0.43	1.90	6	1
1:A:70:TRP:HB3	1:A:79:GLU:HG2	0.42	1.91	2	1
1:A:25:ARG:HH22	1:A:61:GLU:HG2	0.42	1.73	8	1
1:A:13:ILE:HG12	1:A:42:TYR:HB2	0.42	1.91	11	1
1:A:128:ASN:HB2	1:A:132:PHE:CE2	0.42	2.50	17	1
1:A:96:GLU:HB2	1:A:114:LYS:HD2	0.42	1.91	4	1
1:A:68:LYS:HG3	1:A:70:TRP:HZ3	0.42	1.75	1	1
1:A:149:GLU:O	1:A:153:LEU:HG	0.42	2.15	8	1
1:A:58:SER:HB3	1:A:65:TRP:CE2	0.42	2.50	12	1
1:A:146:LEU:O	1:A:151:PRO:HD3	0.42	2.15	16	1
1:A:15:VAL:HB	1:A:131:LYS:HB3	0.42	1.91	2	1
1:A:40:ILE:O	1:A:44:GLU:HG3	0.42	2.15	4	1
1:A:59:ASN:OD1	1:A:61:GLU:HB2	0.42	2.15	19	1
1:A:46:ASN:HD21	1:A:52:ASP:HA	0.42	1.75	14	1
1:A:68:LYS:HE3	1:A:79:GLU:HB2	0.41	1.92	8	1
1:A:117:LEU:HD13	1:A:141:GLY:HA3	0.41	1.92	17	1
1:A:18:THR:HB	1:A:34:GLU:HG3	0.41	1.92	10	1
1:A:26:GLU:HG3	1:A:27:LEU:HD22	0.41	1.92	4	2
1:A:31:ARG:HH21	1:A:91:PRO:HG3	0.41	1.72	14	1
1:A:32:LEU:HG	1:A:36:TYR:CE2	0.41	2.50	5	1
1:A:122:LYS:HB3	1:A:123:PRO:HD3	0.41	1.93	13	2
1:A:44:GLU:HA	1:A:47:LYS:HG2	0.41	1.92	3	1
1:A:39:LEU:O	1:A:43:VAL:HG23	0.41	2.16	15	1
1:A:41:ARG:O	1:A:45:ASN:HB2	0.41	2.15	8	1
1:A:102:LEU:HA	1:A:105:LYS:CD	0.41	2.43	4	1
1:A:6:THR:O	1:A:10:VAL:HG23	0.41	2.15	6	1
1:A:122:LYS:HB2	1:A:123:PRO:CD	0.41	2.45	20	2
1:A:68:LYS:HD2	1:A:70:TRP:CZ2	0.41	2.51	10	1
1:A:153:LEU:HD12	1:A:156:LYS:HD3	0.40	1.93	17	1
1:A:74:ASP:O	1:A:75:LEU:HB2	0.40	2.16	12	1
1:A:118:THR:HG23	1:A:121:PHE:HB2	0.40	1.93	20	1
1:A:125:TRP:CZ3	1:A:137:LEU:HD13	0.40	2.52	15	1
1:A:78:TYR:CE1	1:A:150:ILE:HG21	0.40	2.51	13	1
1:A:18:THR:HG21	1:A:27:LEU:HD12	0.40	1.93	8	1
1:A:51:ASN:C	1:A:51:ASN:HD22	0.40	2.20	6	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	149/175 (85%)	142±2 (95±1%)	6±2 (4±1%)	1±1 (0±1%)	40 79
All	All	2980/3500 (85%)	2841 (95%)	127 (4%)	12 (0%)	40 79

All 5 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	130	PRO	5
1	A	74	ASP	4
1	A	103	ASP	1
1	A	19	ASN	1
1	A	97	ILE	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	131/154 (85%)	126±2 (96±2%)	5±2 (4±2%)	38 84
All	All	2620/3080 (85%)	2515 (96%)	105 (4%)	38 84

All 43 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	36	TYR	8
1	A	79	GLU	7
1	A	41	ARG	6
1	A	32	LEU	6
1	A	53	TRP	5

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Mol	Chain	Res	Type	Models (Total)
1	A	7	ARG	5
1	A	132	PHE	5
1	A	17	LYS	4
1	A	23	ARG	4
1	A	89	THR	4
1	A	55	ARG	3
1	A	48	ASN	3
1	A	74	ASP	3
1	A	101	GLU	3
1	A	44	GLU	3
1	A	31	ARG	3
1	A	114	LYS	2
1	A	103	ASP	2
1	A	56	LEU	2
1	A	83	GLU	2
1	A	60	LYS	2
1	A	149	GLU	2
1	A	64	ARG	1
1	A	118	THR	1
1	A	25	ARG	1
1	A	78	TYR	1
1	A	70	TRP	1
1	A	30	GLN	1
1	A	19	ASN	1
1	A	58	SER	1
1	A	18	THR	1
1	A	54	PHE	1
1	A	38	SER	1
1	A	121	PHE	1
1	A	153	LEU	1
1	A	138	MET	1
1	A	105	LYS	1
1	A	6	THR	1
1	A	51	ASN	1
1	A	85	ASP	1
1	A	128	ASN	1
1	A	45	ASN	1
1	A	33	LYS	1

6.3.3 RNA ⓘ

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