Full wwPDB NMR Structure Validation Report (i)

Mar 6, 2022 – 01:09 PM EST

PDB ID	:	2KF2
Title	:	Solution NMR structure of of Streptomyces coelicolor polyketide cyclase SCO5315. Northeast Structural Genomics Consortium target RR365
Authors	:	Cort, J.R.; Ramelot, T.A.; Ding, K.; Wang, H.; Jiang, M.; Maglaqui, M.; Xiao, R.; Nair, R.; Baran, M.C.; Everett, J.K.; Swapna, G.V.T.; Acton, T.B.; Rost, B.; Montelione, G.T.; Kennedy, M.A.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2009-02-11

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

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

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

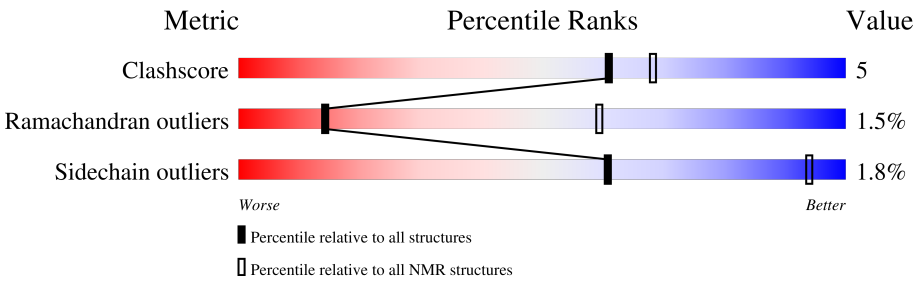
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 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	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	167	84% • • 11%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:2-A:150 (149)	0.60	1

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 and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2638 atoms, of which 1285 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative polyketide cyclase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	167	2638	841	1285	244	259	9	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	THR	ASN	SEE REMARK 999	UNP P23154
A	160	LEU	-	expression tag	UNP P23154
A	161	GLU	-	expression tag	UNP P23154
A	162	HIS	-	expression tag	UNP P23154
A	163	HIS	-	expression tag	UNP P23154
A	164	HIS	-	expression tag	UNP P23154
A	165	HIS	-	expression tag	UNP P23154
A	166	HIS	-	expression tag	UNP P23154
A	167	HIS	-	expression tag	UNP P23154

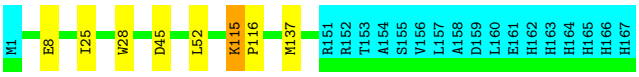
4 Residue-property plots (i)

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: Putative polyketide cyclase

Chain A:



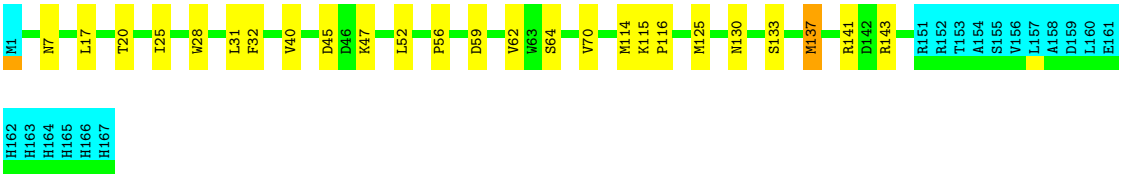
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Putative polyketide cyclase

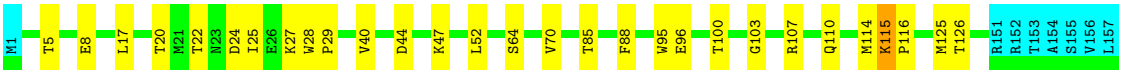
Chain A:

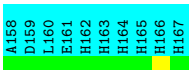


4.2.2 Score per residue for model 2

• Molecule 1: Putative polyketide cyclase

Chain A:

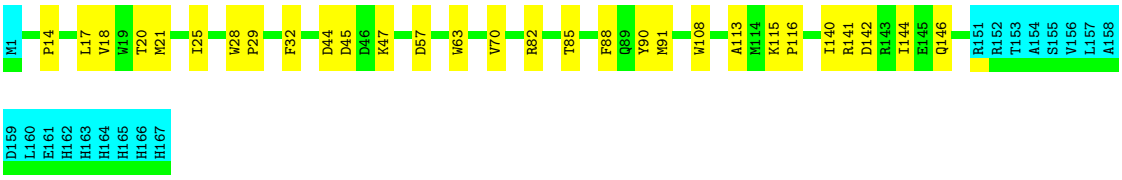




4.2.3 Score per residue for model 3

- Molecule 1: Putative polyketide cyclase

Chain A:



4.2.4 Score per residue for model 4

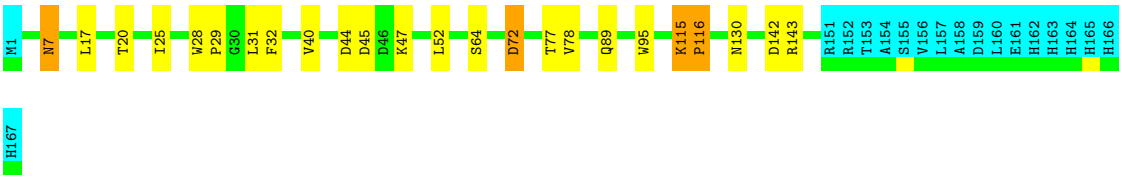
- Molecule 1: Putative polyketide cyclase

Chain A:

4.2.5 Score per residue for model 5

- Molecule 1: Putative polyketide cyclase

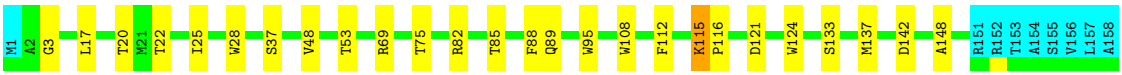
Chain A:

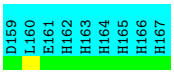


4.2.6 Score per residue for model 6

- Molecule 1: Putative polyketide cyclase

Chain A:





4.2.7 Score per residue for model 7

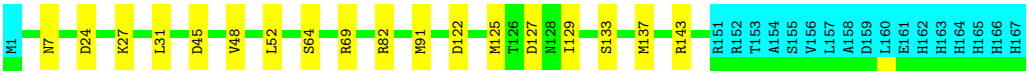
• Molecule 1: Putative polyketide cyclase

Chain A:

4.2.8 Score per residue for model 8

• Molecule 1: Putative polyketide cyclase

Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Putative polyketide cyclase

Chain A:

4.2.10 Score per residue for model 10

• Molecule 1: Putative polyketide cyclase

Chain A:

4.2.11 Score per residue for model 11

• Molecule 1: Putative polyketide cyclase

Chain A: 77% 12% • 11%

M1 N23 L31 F32 K47 F50 P56 D57 V62 W63 S67 E68 R69 V70 R76 T77 V78 A98 E99 T100 V105 K115 P116 R143 R151 R152 T153 A154 S155 V156 L157 A158 D159 L160 E161 H162 H163 H164 H165 H166 H167

4.2.12 Score per residue for model 12

- Molecule 1: Putative polyketide cyclase

Chain A: 80% 8% • 11%

M1 M15 E16 L17 T20 I25 W28 L52 S64 W65 M91 E99 W108 F112 K115 P116 R141 R151 R152 T153 A154 S155 V156 L157 A158 D159 L160 E161 H162 H163 H164 H165 H166 H167

4.2.13 Score per residue for model 13

- Molecule 1: Putative polyketide cyclase

Chain A: 74% 15% • 11%

M1 E8 E16 I25 W28 P29 E34 E39 V48 R51 R69 Y90 E96 M106 R107 A113 M114 K115 P116 M125 T126 D127 N132 S133 Q136 M137 D142 Q146 R151 R152 T153 A154 S155 V156 L157 A158 D159 L160 E161 H162 H163 H164 H165 H166 H167

4.2.14 Score per residue for model 14

- Molecule 1: Putative polyketide cyclase

Chain A: 80% 10% 11%

M1 N7 E8 W28 P29 F32 D45 L52 W63 S64 W65 T75 T85 R107 W108 K115 R134 R151 R152 T153 A154 S155 V156 L157 A158 D159 L160 E161 H162 H163 H164 H165 H166 H167

4.2.15 Score per residue for model 15

- Molecule 1: Putative polyketide cyclase

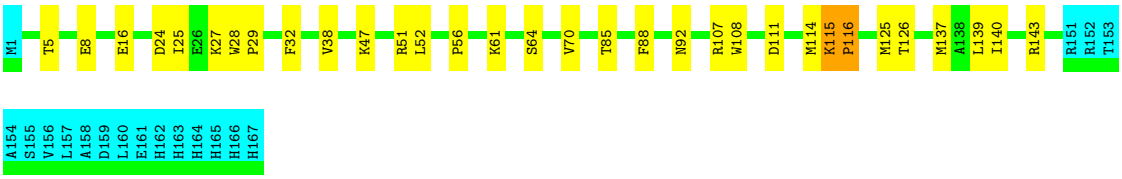
Chain A: 77% 11% • 11%

M1 N7 E8 M15 R43 D44 D45 V48 L52 S64 E68 A80 T85 F88 E96 E99 R107 W108 K115 P116 D122 N130 D142 R151 R152 T153 A154 S155 V156 L157 A158 D159 L160 E161 H162 H163 H164 H165 H166 H167

4.2.16 Score per residue for model 16

- Molecule 1: Putative polyketide cyclase

Chain A: 70% 18% • 11%



4.2.17 Score per residue for model 17

- Molecule 1: Putative polyketide cyclase

Chain A: 77% 12% • 11%

4.2.18 Score per residue for model 18

- Molecule 1: Putative polyketide cyclase

Chain A: 77% 12% • 11%

4.2.19 Score per residue for model 19

- Molecule 1: Putative polyketide cyclase

Chain A: 77% 12% • 11%

4.2.20 Score per residue for model 20

- Molecule 1: Putative polyketide cyclase

Chain A: 76% 13% • 11%

M1
N7
E8
I9
D24
I25
W28
P29
V38
D45
D46
K47
L52
W65
V70
A71
D72
R82
N92
W108
T109
Q110
D111
K115
P116
D117
M137
R151
R152
T153
A154
S155
V156
L157
A158
D159
L160
E161
H162
H163
H164
H165
H166
H167

5 Refinement protocol and experimental data overview (i)

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

Of the 40 calculated structures, 20 were deposited, based on the following criterion: *lowest energy, fewest restraint violations, favorable backbone geometry.*

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

Software name	Classification	Version
AutoStructure	structure solution	.
CNS	refinement	.
X-PLOR NIH	refinement	.
PSVS	structure solution	.

No chemical shift data was provided.

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	1199	1137	1135	11±3
All	All	23980	22740	22700	215

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:31:LEU:HG	1:A:143:ARG:HG2	0.83	1.48	5	3
1:A:8:GLU:HG2	1:A:107:ARG:HG2	0.76	1.56	19	8
1:A:24:ASP:HB2	1:A:27:LYS:HE2	0.74	1.58	8	1
1:A:115:LYS:HA	1:A:115:LYS:HE3	0.71	1.61	19	1
1:A:114:MET:SD	1:A:125:MET:HG3	0.70	2.26	4	4
1:A:47:LYS:HG2	1:A:70:VAL:HG22	0.66	1.64	2	7
1:A:9:ILE:HG13	1:A:137:MET:HB3	0.66	1.65	20	1
1:A:52:LEU:O	1:A:64:SER:HA	0.64	1.92	16	10
1:A:7:ASN:HB2	1:A:108:TRP:HB2	0.63	1.71	20	2
1:A:48:VAL:HG13	1:A:69:ARG:HB3	0.62	1.70	13	3
1:A:44:ASP:HB3	1:A:47:LYS:HB2	0.62	1.72	2	2
1:A:15:MET:SD	1:A:99:GLU:HB2	0.62	2.34	15	1
1:A:96:GLU:HB2	1:A:107:ARG:HB2	0.62	1.72	2	1
1:A:89:GLN:HB2	1:A:115:LYS:HB2	0.61	1.69	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:LYS:HB3	1:A:116:PRO:HD3	0.61	1.72	5	4
1:A:44:ASP:HB2	1:A:47:LYS:HB2	0.61	1.70	17	2
1:A:89:GLN:HG3	1:A:115:LYS:HD2	0.60	1.73	6	1
1:A:17:LEU:HA	1:A:20:THR:HG22	0.60	1.73	12	4
1:A:56:PRO:HB3	1:A:62:VAL:HG22	0.59	1.72	17	2
1:A:17:LEU:HD23	1:A:148:ALA:HB1	0.59	1.75	19	1
1:A:56:PRO:HG3	1:A:62:VAL:HG22	0.58	1.74	19	2
1:A:115:LYS:N	1:A:116:PRO:HD2	0.58	2.14	9	4
1:A:85:THR:HG22	1:A:88:PHE:HB2	0.58	1.74	18	2
1:A:7:ASN:HD21	1:A:129:ILE:HG22	0.58	1.59	4	1
1:A:133:SER:O	1:A:137:MET:HG2	0.57	1.99	9	4
1:A:108:TRP:HB3	1:A:110:GLN:HE21	0.57	1.59	20	1
1:A:85:THR:HB	1:A:88:PHE:O	0.57	1.99	2	4
1:A:7:ASN:OD1	1:A:130:ASN:HA	0.55	2.00	5	4
1:A:90:TYR:HB3	1:A:113:ALA:HB3	0.55	1.78	10	4
1:A:5:THR:HG23	1:A:126:THR:HG23	0.55	1.79	16	1
1:A:92:ASN:HB3	1:A:111:ASP:HB2	0.55	1.79	20	1
1:A:92:ASN:HB3	1:A:111:ASP:HB3	0.53	1.81	16	1
1:A:133:SER:O	1:A:137:MET:HB2	0.52	2.05	1	1
1:A:85:THR:HG21	1:A:88:PHE:HB2	0.52	1.80	17	2
1:A:3:GLY:HA3	1:A:112:PHE:CE1	0.52	2.40	6	1
1:A:125:MET:O	1:A:129:ILE:HG12	0.52	2.05	8	1
1:A:39:GLU:HB3	1:A:51:ARG:HB3	0.52	1.82	10	1
1:A:25:ILE:HG22	1:A:28:TRP:CZ2	0.51	2.40	10	11
1:A:69:ARG:HA	1:A:79:ARG:O	0.51	2.04	10	1
1:A:15:MET:SD	1:A:99:GLU:HG2	0.51	2.46	12	1
1:A:4:HIS:HB3	1:A:111:ASP:HA	0.50	1.81	9	1
1:A:85:THR:CG2	1:A:88:PHE:HB2	0.50	2.36	18	3
1:A:28:TRP:N	1:A:29:PRO:HD2	0.50	2.22	18	10
1:A:57:ASP:HB2	1:A:63:TRP:CZ2	0.50	2.41	3	1
1:A:115:LYS:N	1:A:116:PRO:CD	0.50	2.74	18	2
1:A:24:ASP:HB2	1:A:27:LYS:HD2	0.50	1.83	19	1
1:A:7:ASN:HD21	1:A:134:ARG:HB2	0.50	1.66	14	1
1:A:115:LYS:NZ	1:A:115:LYS:HB3	0.50	2.22	18	1
1:A:8:GLU:HG2	1:A:107:ARG:HG3	0.49	1.85	4	1
1:A:7:ASN:ND2	1:A:133:SER:HB2	0.49	2.21	8	1
1:A:8:GLU:HG2	1:A:107:ARG:HD2	0.49	1.83	17	1
1:A:115:LYS:HB2	1:A:116:PRO:HD3	0.48	1.84	6	1
1:A:142:ASP:O	1:A:146:GLN:HG3	0.48	2.09	3	2
1:A:17:LEU:HA	1:A:20:THR:HB	0.48	1.86	3	5
1:A:137:MET:SD	1:A:140:ILE:HD12	0.48	2.49	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:THR:HB	1:A:95:TRP:HZ3	0.47	1.69	6	2
1:A:4:HIS:HA	1:A:110:GLN:O	0.47	2.09	9	1
1:A:82:ARG:HH21	1:A:85:THR:HG23	0.47	1.69	6	1
1:A:23:ASN:HA	1:A:69:ARG:NH2	0.47	2.24	11	1
1:A:132:ASN:O	1:A:136:GLN:HG2	0.47	2.09	13	1
1:A:25:ILE:HB	1:A:38:VAL:HG11	0.47	1.87	17	1
1:A:7:ASN:ND2	1:A:108:TRP:HB2	0.46	2.26	19	1
1:A:114:MET:O	1:A:115:LYS:HB2	0.46	2.10	4	2
1:A:96:GLU:HB3	1:A:107:ARG:HB2	0.46	1.87	15	3
1:A:52:LEU:HD13	1:A:65:TRP:CZ2	0.46	2.45	20	1
1:A:43:ARG:HB3	1:A:48:VAL:HG23	0.46	1.87	9	2
1:A:63:TRP:HB3	1:A:65:TRP:CZ3	0.46	2.46	14	1
1:A:114:MET:C	1:A:116:PRO:HD2	0.45	2.32	2	1
1:A:50:PHE:CZ	1:A:67:SER:HB2	0.45	2.47	11	1
1:A:57:ASP:HB2	1:A:63:TRP:CH2	0.45	2.47	11	1
1:A:38:VAL:HG22	1:A:52:LEU:HG	0.45	1.89	20	1
1:A:82:ARG:HD2	1:A:91:MET:SD	0.44	2.52	8	1
1:A:121:ASP:H	1:A:124:TRP:HD1	0.44	1.56	6	2
1:A:50:PHE:CE1	1:A:69:ARG:HB2	0.44	2.47	19	1
1:A:17:LEU:HD23	1:A:148:ALA:HB2	0.44	1.89	6	1
1:A:72:ASP:HB3	1:A:77:THR:O	0.44	2.13	5	1
1:A:25:ILE:HD11	1:A:40:VAL:HG22	0.43	1.90	1	3
1:A:137:MET:HE2	1:A:137:MET:HA	0.43	1.91	13	2
1:A:56:PRO:HA	1:A:61:LYS:O	0.43	2.12	16	1
1:A:7:ASN:HD22	1:A:133:SER:HB2	0.43	1.73	8	1
1:A:70:VAL:O	1:A:78:VAL:HA	0.43	2.13	10	1
1:A:14:PRO:O	1:A:18:VAL:HG23	0.43	2.14	3	1
1:A:125:MET:HA	1:A:125:MET:CE	0.43	2.43	2	1
1:A:139:LEU:O	1:A:143:ARG:HG2	0.43	2.14	16	1
1:A:50:PHE:CE1	1:A:67:SER:HB2	0.43	2.49	18	1
1:A:23:ASN:HA	1:A:69:ARG:HH12	0.42	1.74	19	1
1:A:5:THR:OG1	1:A:110:GLN:HB2	0.42	2.14	2	1
1:A:24:ASP:OD2	1:A:27:LYS:HG2	0.42	2.14	2	1
1:A:98:ALA:HB3	1:A:105:VAL:HB	0.42	1.90	11	1
1:A:91:MET:SD	1:A:112:PHE:HB3	0.42	2.54	12	1
1:A:100:THR:HB	1:A:103:GLY:O	0.42	2.15	2	1
1:A:137:MET:O	1:A:141:ARG:HB2	0.42	2.14	1	1
1:A:78:VAL:HB	1:A:95:TRP:HB2	0.42	1.91	5	1
1:A:89:GLN:CG	1:A:115:LYS:HD2	0.42	2.44	6	1
1:A:39:GLU:HB2	1:A:51:ARG:HB3	0.42	1.90	13	2
1:A:32:PHE:HE1	1:A:136:GLN:HB3	0.42	1.75	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ILE:HA	1:A:28:TRP:CD1	0.42	2.50	17	2
1:A:82:ARG:HB3	1:A:91:MET:HB2	0.42	1.91	17	1
1:A:82:ARG:HH21	1:A:91:MET:HG3	0.42	1.75	3	1
1:A:37:SER:HB2	1:A:53:THR:HB	0.42	1.92	6	1
1:A:48:VAL:CG1	1:A:69:ARG:HB3	0.41	2.44	13	1
1:A:133:SER:O	1:A:137:MET:HG3	0.41	2.15	8	1
1:A:51:ARG:HG2	1:A:64:SER:HB2	0.41	1.90	16	1
1:A:24:ASP:OD2	1:A:27:LYS:HG3	0.41	2.16	16	1
1:A:17:LEU:O	1:A:21:MET:HG2	0.41	2.16	3	1
1:A:125:MET:O	1:A:129:ILE:HG13	0.41	2.14	9	1
1:A:28:TRP:HB2	1:A:38:VAL:HG21	0.41	1.93	16	1
1:A:129:ILE:O	1:A:133:SER:HB2	0.41	2.16	9	1
1:A:115:LYS:H	1:A:116:PRO:CD	0.41	2.29	7	1
1:A:112:PHE:HE2	1:A:122:ASP:HA	0.41	1.76	9	1
1:A:90:TYR:O	1:A:112:PHE:HA	0.41	2.15	10	1
1:A:76:ARG:NH1	1:A:99:GLU:HB2	0.41	2.31	11	1
1:A:68:GLU:O	1:A:80:ALA:HA	0.41	2.16	15	1
1:A:115:LYS:H	1:A:116:PRO:HD2	0.41	1.76	15	1
1:A:5:THR:CG2	1:A:126:THR:HA	0.40	2.46	2	1
1:A:31:LEU:HG	1:A:143:ARG:HG3	0.40	1.93	8	1
1:A:140:ILE:O	1:A:144:ILE:HG12	0.40	2.16	3	1
1:A:89:GLN:HE21	1:A:115:LYS:HB2	0.40	1.76	10	1
1:A:96:GLU:O	1:A:106:MET:HA	0.40	2.16	13	1
1:A:69:ARG:CZ	1:A:78:VAL:HG11	0.40	2.47	11	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	149/167 (89%)	140±2 (94±1%)	6±2 (4±1%)	2±1 (2±1%)	14	59
All	All	2980/3340 (89%)	2807 (94%)	127 (4%)	46 (2%)	14	59

All 7 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	115	LYS	19
1	A	45	ASP	13
1	A	116	PRO	7
1	A	122	ASP	3
1	A	34	GLU	2
1	A	16	GLU	1
1	A	85	THR	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	127/143 (89%)	125±1 (98±1%)	2±1 (2±1%)	61 94
All	All	2540/2860 (89%)	2495 (98%)	45 (2%)	61 94

All 25 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	32	PHE	7
1	A	108	TRP	5
1	A	137	MET	4
1	A	142	ASP	3
1	A	59	ASP	2
1	A	141	ARG	2
1	A	72	ASP	2
1	A	75	THR	2
1	A	127	ASP	2
1	A	20	THR	1
1	A	7	ASN	1
1	A	54	MET	1
1	A	8	GLU	1
1	A	23	ASN	1
1	A	100	THR	1
1	A	65	TRP	1
1	A	85	THR	1
1	A	16	GLU	1
1	A	47	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	79	ARG	1
1	A	128	ASN	1
1	A	115	LYS	1
1	A	24	ASP	1
1	A	82	ARG	1
1	A	117	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 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)

No chemical shift data were provided