Full wwPDB NMR Structure Validation Report (i)

Feb 26, 2022 – 12:16 PM EST

PDB ID	:	2CRJ
Title	:	Solution structure of the HMG domain of mouse HMG domain protein HMGX2
Authors	:	Endo, H.; Hayashi, F.; Yoshida, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-05-20

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:

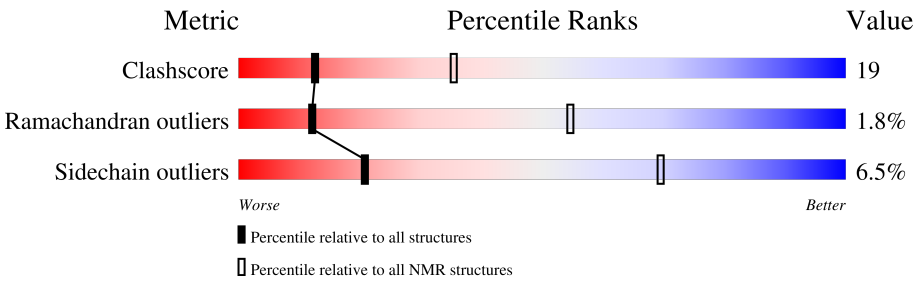
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	92	43% 24% • 29%

2 Ensemble composition and analysis (i)

This entry contains 20 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:8-A:72 (65)	0.34	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 3 clusters and 5 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1462 atoms, of which 722 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	92	1462	464	722	130	144	2	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q9Z104
A	2	SER	-	cloning artifact	UNP Q9Z104
A	3	SER	-	cloning artifact	UNP Q9Z104
A	4	GLY	-	cloning artifact	UNP Q9Z104
A	5	SER	-	cloning artifact	UNP Q9Z104
A	6	SER	-	cloning artifact	UNP Q9Z104
A	7	GLY	-	cloning artifact	UNP Q9Z104
A	87	SER	-	cloning artifact	UNP Q9Z104
A	88	GLY	-	cloning artifact	UNP Q9Z104
A	89	PRO	-	cloning artifact	UNP Q9Z104
A	90	SER	-	cloning artifact	UNP Q9Z104
A	91	SER	-	cloning artifact	UNP Q9Z104
A	92	GLY	-	cloning artifact	UNP Q9Z104

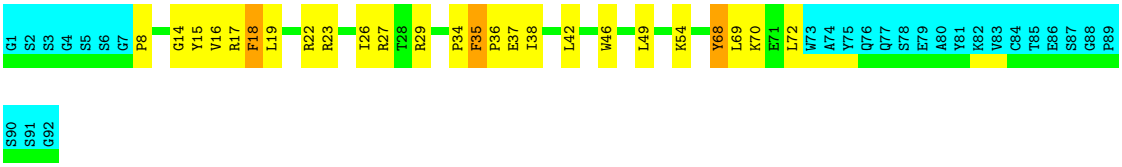
4 Residue-property plots (i)

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: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

Chain A: 43% 24% • 29%



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: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

Chain A: 36% 32% • 29%

4.2.2 Score per residue for model 2

• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

Chain A: 43% 21% 7% 29%

G1 S2 S3 G4 S5 S6 G7 A10 T13 G14 F18 R22 I26 R27 T28 R29 H30 P31 D32 L33 P34 F35 P36 E37 I38 W46 L49 K54 K65 Q66 Q67 Y68 L69 K70 W73 A74 Y75 Q76 Q77 S78 E79 A80 Y81 K82 V83 C84 T85 E86 S87 G88

P89 S90 S91 G92

4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

Chain A: 43% 22% 5% 29%

G1 S2 S3 G4 S5 S6 G7 P8 K9 A10 T13 G14 Y15 V16 R17 F18 L19 N20 I26 R27 T28 R29 P34 F35 P36 E37 I38 W46 L49 K54 Q66 Q67 Y68 L69 K70 E71 L72 W73 A74 Y75 Q76 Q77 S78 E79 A80 Y81 K82 V83 C84 T85 E86 S87 G88

P89 S90 S91 G92

4.2.4 Score per residue for model 4

• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

Chain A: 43% 24% • 29%

G1 S2 S3 G4 S5 S6 G7 P8 Y15 V16 R17 F18 L19 R22 Q25 I26 D32 L33 P34 F35 P36 E37 I38 L42 G43 A44 E45 W46 L49 K54 Y68 L69 K70 W73 A74 Y75 Q76 Q77 S78 E79 A80 Y81 K82 V83 C84 T85 E86 S87 G88 P89 S90

S91 G92

4.2.5 Score per residue for model 5

• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

Chain A: 39% 28% • 29%

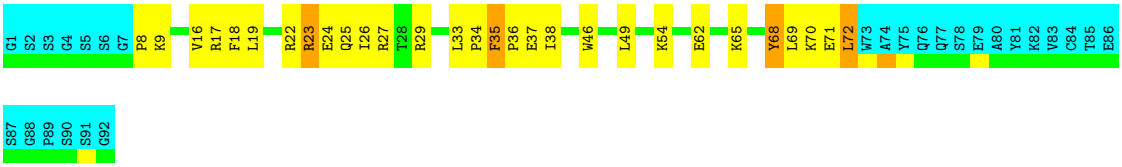
G1 S2 S3 G4 S5 S6 G7 P8 K9 G14 Y15 V16 R17 F18 L19 N20 E21 R22 R23 I26 R27 T28 R29 P34 F35 P36 E37 I38 L42 W46 L49 Q55 L58 D59 E60 A61 E62 K65 Q66 Q67 Y68 L69 K70 W73 A74 Y75 Q76 Q77 S78 E79

A80 Y81 K82 V83 C84 T85 E86 S87 G88 P89 S90 S91 G92

4.2.6 Score per residue for model 6

• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

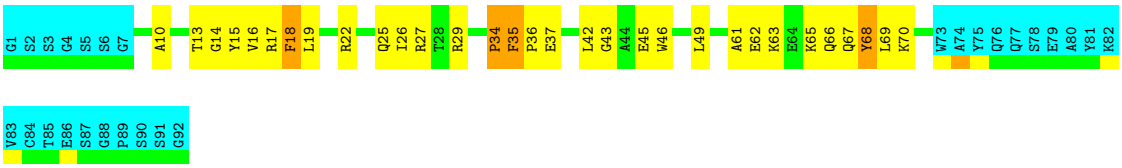
Chain A: 39% 27% • 29%



4.2.7 Score per residue for model 7

• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

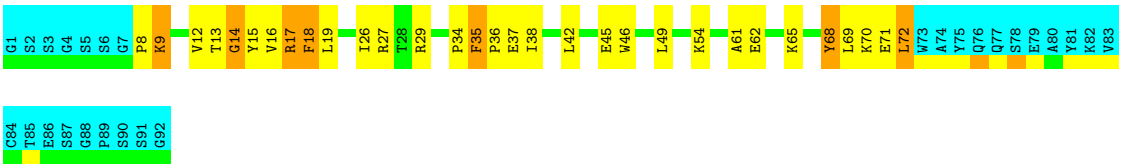
Chain A: 37% 29% • 29%



4.2.8 Score per residue for model 8

• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

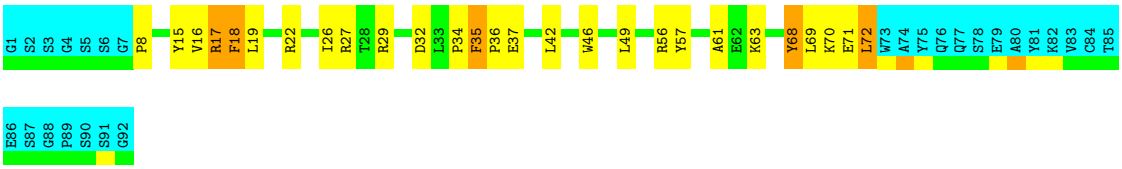
Chain A: 37% 26% 8% 29%



4.2.9 Score per residue for model 9

• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

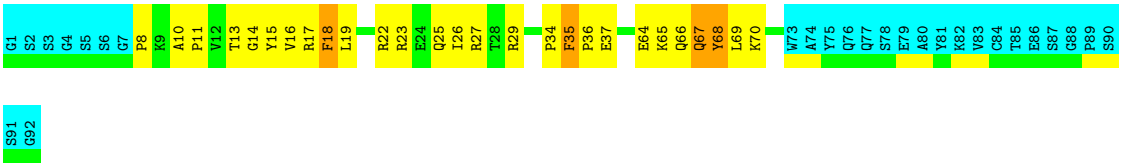
Chain A: 41% 24% 5% 29%



4.2.10 Score per residue for model 10

• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

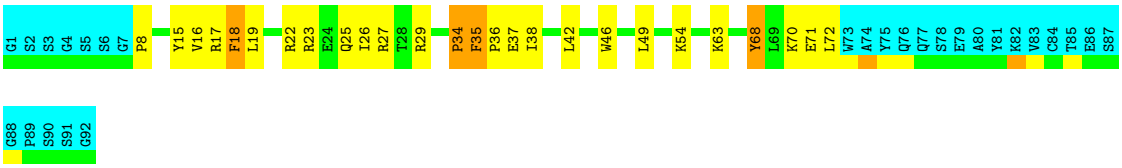
Chain A: 41% 25% • 29%



4.2.11 Score per residue for model 11

• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

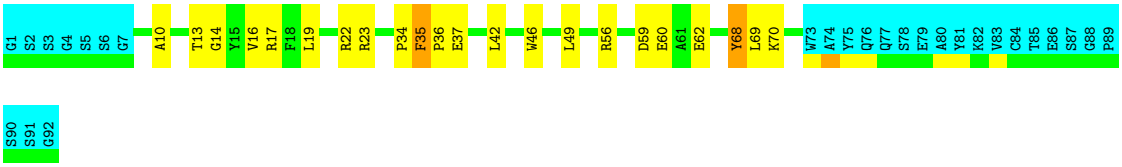
Chain A: 42% 24% • 29%



4.2.12 Score per residue for model 12

• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

Chain A: 47% 22% • 29%



4.2.13 Score per residue for model 13

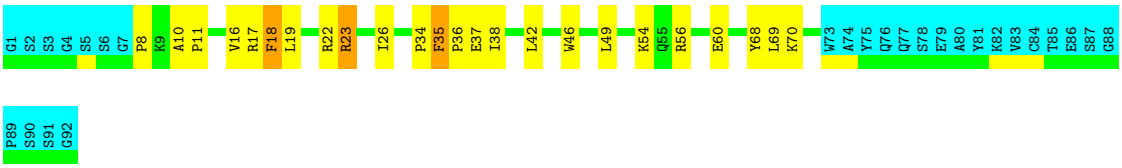
• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

Chain A: 45% 23% • 29%

4.2.14 Score per residue for model 14

• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

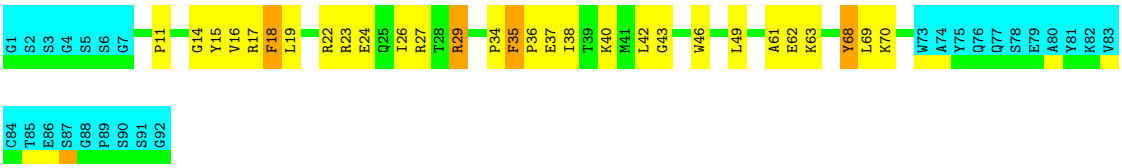
Chain A: 45% 23% • 29%



4.2.15 Score per residue for model 15

• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

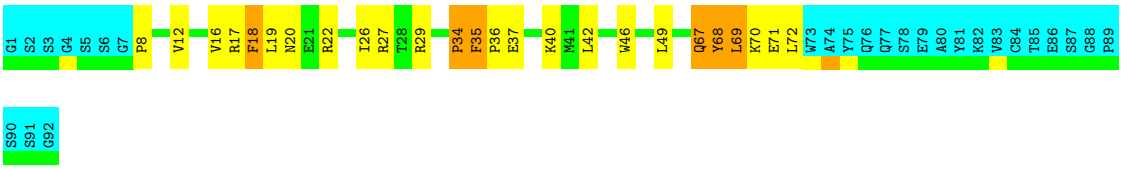
Chain A: 39% 27% • 29%



4.2.16 Score per residue for model 16

• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

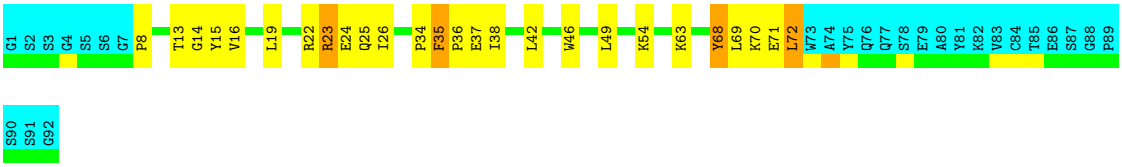
Chain A: 43% 21% 7% 29%



4.2.17 Score per residue for model 17

• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

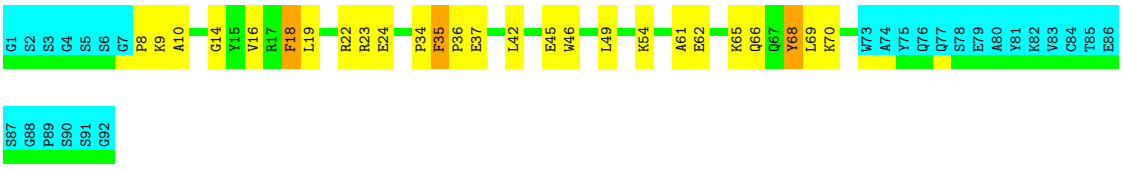
Chain A: 42% 24% • 29%



4.2.18 Score per residue for model 18

• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

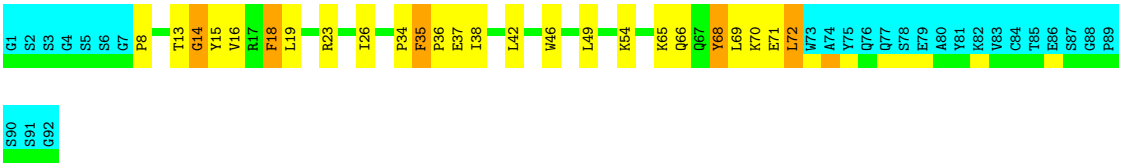
Chain A: 42% 25% • 29%



4.2.19 Score per residue for model 19

• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

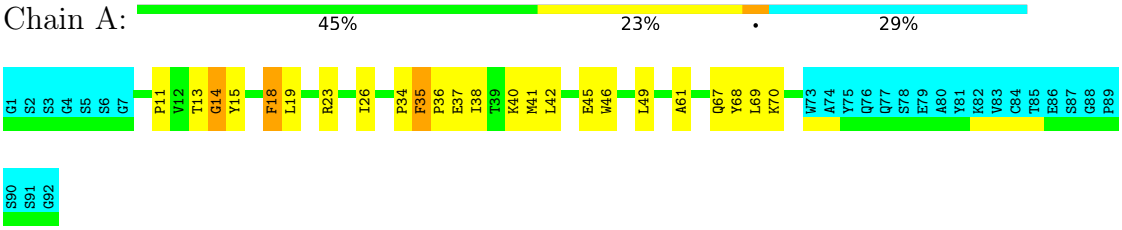
Chain A: 43% 22% 5% 29%



4.2.20 Score per residue for model 20

• Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1-related

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function, structures with the lowest energy, structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

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	552	560	559	21±3
All	All	11040	11200	11180	417

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ARG:HD2	1:A:61:ALA:HB2	0.76	1.55	8	2
1:A:12:VAL:HG23	1:A:17:ARG:HG3	0.70	1.62	16	1
1:A:66:GLN:HA	1:A:69:LEU:HD12	0.67	1.63	18	1
1:A:46:TRP:CE3	1:A:49:LEU:HD12	0.66	2.26	16	19
1:A:12:VAL:HG11	1:A:20:ASN:HD21	0.65	1.52	1	1
1:A:35:PHE:C	1:A:35:PHE:CD1	0.63	2.72	16	18
1:A:16:VAL:HG12	1:A:20:ASN:OD1	0.62	1.95	5	1
1:A:16:VAL:HA	1:A:19:LEU:HD12	0.62	1.72	17	5
1:A:23:ARG:HD2	1:A:38:ILE:HG21	0.61	1.71	11	1
1:A:26:ILE:HG21	1:A:38:ILE:HG23	0.60	1.73	4	13
1:A:55:GLN:OE1	1:A:58:LEU:HD12	0.60	1.97	5	1
1:A:16:VAL:HG12	1:A:20:ASN:ND2	0.59	2.12	13	3
1:A:15:TYR:CZ	1:A:19:LEU:HD11	0.58	2.34	15	9
1:A:26:ILE:CG1	1:A:42:LEU:HD21	0.58	2.29	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:ARG:HB3	1:A:42:LEU:HD22	0.58	1.74	9	6
1:A:26:ILE:CG2	1:A:38:ILE:HG23	0.54	2.32	4	3
1:A:18:PHE:C	1:A:18:PHE:CD1	0.53	2.82	15	6
1:A:10:ALA:N	1:A:68:TYR:CE2	0.52	2.78	18	2
1:A:68:TYR:CD1	1:A:68:TYR:C	0.52	2.83	17	14
1:A:68:TYR:CD1	1:A:69:LEU:N	0.52	2.78	9	3
1:A:46:TRP:CH2	1:A:54:LYS:HG2	0.52	2.40	2	10
1:A:11:PRO:HD3	1:A:68:TYR:CD1	0.52	2.40	14	1
1:A:67:GLN:CD	1:A:67:GLN:C	0.51	2.70	10	1
1:A:62:GLU:CG	1:A:63:LYS:N	0.51	2.74	7	1
1:A:26:ILE:O	1:A:29:ARG:N	0.50	2.45	3	13
1:A:14:GLY:N	1:A:61:ALA:CB	0.50	2.74	7	6
1:A:16:VAL:O	1:A:19:LEU:N	0.50	2.45	6	10
1:A:22:ARG:O	1:A:24:GLU:N	0.50	2.45	17	3
1:A:42:LEU:O	1:A:45:GLU:N	0.50	2.45	7	6
1:A:13:THR:O	1:A:16:VAL:N	0.50	2.45	8	4
1:A:16:VAL:HG12	1:A:20:ASN:HD22	0.49	1.67	13	1
1:A:22:ARG:O	1:A:25:GLN:N	0.49	2.46	11	5
1:A:18:PHE:CD1	1:A:18:PHE:C	0.49	2.86	16	7
1:A:10:ALA:HA	1:A:68:TYR:CE2	0.49	2.42	2	7
1:A:56:ARG:O	1:A:60:GLU:CG	0.49	2.60	14	1
1:A:65:LYS:CG	1:A:69:LEU:CD2	0.49	2.90	5	1
1:A:71:GLU:O	1:A:72:LEU:C	0.48	2.52	6	8
1:A:15:TYR:CE1	1:A:19:LEU:HD11	0.48	2.43	15	1
1:A:8:PRO:HB2	1:A:68:TYR:CD2	0.48	2.43	16	10
1:A:35:PHE:N	1:A:36:PRO:HD2	0.48	2.23	9	20
1:A:65:LYS:O	1:A:67:GLN:N	0.47	2.48	2	2
1:A:65:LYS:O	1:A:68:TYR:N	0.47	2.48	2	1
1:A:11:PRO:HD3	1:A:68:TYR:CD2	0.47	2.44	10	4
1:A:62:GLU:O	1:A:65:LYS:N	0.47	2.47	18	3
1:A:18:PHE:CZ	1:A:22:ARG:HG3	0.47	2.44	6	5
1:A:23:ARG:O	1:A:26:ILE:N	0.46	2.48	15	1
1:A:10:ALA:HA	1:A:68:TYR:CD2	0.46	2.46	3	1
1:A:35:PHE:CD1	1:A:35:PHE:C	0.46	2.89	12	2
1:A:14:GLY:CA	1:A:61:ALA:HB2	0.46	2.41	5	1
1:A:8:PRO:HG2	1:A:68:TYR:CE2	0.46	2.45	8	5
1:A:26:ILE:O	1:A:27:ARG:C	0.45	2.55	3	12
1:A:13:THR:O	1:A:14:GLY:C	0.45	2.55	3	10
1:A:22:ARG:O	1:A:23:ARG:C	0.45	2.55	10	7
1:A:17:ARG:CZ	1:A:17:ARG:CB	0.45	2.94	9	1
1:A:8:PRO:HB2	1:A:68:TYR:CD1	0.45	2.46	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:GLU:O	1:A:65:LYS:C	0.45	2.54	10	1
1:A:18:PHE:CE2	1:A:22:ARG:HG3	0.45	2.47	2	2
1:A:23:ARG:HA	1:A:42:LEU:HD11	0.45	1.87	20	3
1:A:22:ARG:HB2	1:A:42:LEU:HD13	0.45	1.87	11	1
1:A:70:LYS:O	1:A:71:GLU:C	0.44	2.56	8	1
1:A:59:ASP:O	1:A:62:GLU:N	0.44	2.50	12	2
1:A:16:VAL:CG1	1:A:20:ASN:ND2	0.44	2.80	13	1
1:A:69:LEU:O	1:A:70:LYS:C	0.44	2.56	16	1
1:A:23:ARG:N	1:A:42:LEU:HD11	0.44	2.26	11	1
1:A:46:TRP:CE2	1:A:54:LYS:HE2	0.44	2.48	14	2
1:A:16:VAL:O	1:A:17:ARG:C	0.44	2.56	14	8
1:A:70:LYS:HG3	1:A:71:GLU:N	0.44	2.27	11	1
1:A:22:ARG:CB	1:A:42:LEU:HD22	0.44	2.43	12	2
1:A:65:LYS:O	1:A:66:GLN:C	0.43	2.55	2	4
1:A:65:LYS:CG	1:A:69:LEU:HD21	0.43	2.42	5	1
1:A:70:LYS:CG	1:A:71:GLU:N	0.43	2.81	11	1
1:A:67:GLN:O	1:A:70:LYS:CG	0.43	2.66	1	2
1:A:34:PRO:HG2	1:A:37:GLU:CG	0.43	2.43	11	19
1:A:12:VAL:HG21	1:A:17:ARG:HB3	0.43	1.90	8	1
1:A:66:GLN:O	1:A:69:LEU:N	0.43	2.51	10	1
1:A:42:LEU:O	1:A:43:GLY:C	0.43	2.57	15	4
1:A:17:ARG:CZ	1:A:17:ARG:HB2	0.43	2.43	9	1
1:A:35:PHE:CB	1:A:36:PRO:CD	0.43	2.97	6	20
1:A:26:ILE:O	1:A:28:THR:N	0.43	2.52	2	1
1:A:26:ILE:HG23	1:A:41:MET:CE	0.43	2.44	20	1
1:A:14:GLY:HA2	1:A:61:ALA:HB2	0.43	1.90	5	1
1:A:22:ARG:C	1:A:24:GLU:N	0.43	2.71	17	3
1:A:13:THR:O	1:A:15:TYR:N	0.43	2.51	19	3
1:A:34:PRO:CG	1:A:37:GLU:HG3	0.42	2.44	18	7
1:A:59:ASP:O	1:A:60:GLU:C	0.42	2.57	12	1
1:A:62:GLU:O	1:A:63:LYS:C	0.42	2.57	15	1
1:A:29:ARG:O	1:A:31:PRO:CD	0.42	2.68	2	1
1:A:46:TRP:CE3	1:A:49:LEU:CD1	0.42	3.02	19	2
1:A:34:PRO:CD	1:A:37:GLU:HB2	0.42	2.45	13	8
1:A:18:PHE:O	1:A:22:ARG:CG	0.42	2.68	5	1
1:A:15:TYR:CE2	1:A:19:LEU:HD11	0.42	2.49	9	1
1:A:35:PHE:CD2	1:A:36:PRO:HD3	0.41	2.50	6	1
1:A:23:ARG:O	1:A:24:GLU:C	0.41	2.57	15	1
1:A:65:LYS:C	1:A:67:GLN:N	0.41	2.73	7	1
1:A:65:LYS:HG3	1:A:69:LEU:CD2	0.41	2.44	5	1
1:A:22:ARG:NH1	1:A:25:GLN:OE1	0.41	2.53	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ARG:HD2	1:A:38:ILE:CG2	0.41	2.43	11	1
1:A:19:LEU:O	1:A:23:ARG:N	0.41	2.53	19	1
1:A:33:LEU:HD22	1:A:37:GLU:HB3	0.41	1.91	1	4
1:A:16:VAL:O	1:A:18:PHE:N	0.41	2.54	8	1
1:A:10:ALA:CA	1:A:68:TYR:CE2	0.41	3.04	18	1
1:A:45:GLU:O	1:A:48:LYS:N	0.41	2.54	1	1
1:A:9:LYS:C	1:A:68:TYR:CE2	0.41	2.94	5	2
1:A:56:ARG:NH2	1:A:57:TYR:CE1	0.40	2.90	9	1
1:A:27:ARG:HG2	1:A:38:ILE:HD13	0.40	1.92	11	1
1:A:46:TRP:CE2	1:A:54:LYS:HE3	0.40	2.52	6	2
1:A:62:GLU:HG3	1:A:63:LYS:N	0.40	2.32	7	1
1:A:66:GLN:O	1:A:67:GLN:C	0.40	2.59	3	1
1:A:10:ALA:HA	1:A:68:TYR:CE1	0.40	2.52	14	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	65/92 (71%)	55±3 (85±4%)	9±3 (14±4%)	1±1 (2±2%)	12	54
All	All	1300/1840 (71%)	1099 (85%)	178 (14%)	23 (2%)	12	54

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	14	GLY	6
1	A	72	LEU	6
1	A	23	ARG	3
1	A	34	PRO	3
1	A	66	GLN	2
1	A	27	ARG	1
1	A	9	LYS	1
1	A	69	LEU	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	59/79 (75%)	55±1 (93±2%)	4±1 (7±2%)	21	69
All	All	1180/1580 (75%)	1103 (93%)	77 (7%)	21	69

All 15 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	35	PHE	20
1	A	68	TYR	18
1	A	18	PHE	16
1	A	63	LYS	4
1	A	67	GLN	3
1	A	40	LYS	3
1	A	32	ASP	2
1	A	9	LYS	2
1	A	17	ARG	2
1	A	23	ARG	2
1	A	25	GLN	1
1	A	70	LYS	1
1	A	66	GLN	1
1	A	56	ARG	1
1	A	29	ARG	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