Full wwPDB NMR Structure Validation Report (i)

Feb 26, 2022 – 03:36 PM EST

PDB ID	:	2CRU
Title	:	Solution structure of programmed cell death 5
Authors	:	Nagashima, T.; Izumi, K.; 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:

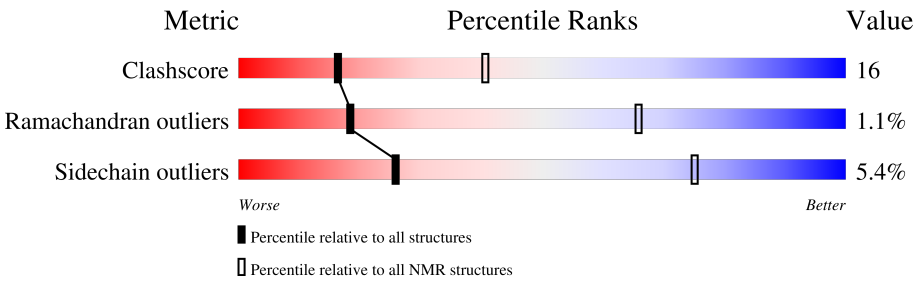
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	118	37% 15% 47%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 13 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:37-A:98 (62)	0.31	13

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 5 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1835 atoms, of which 930 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Programmed cell death protein 5.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	118	1835	550	930	174	179	2	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP O14737
A	2	SER	-	cloning artifact	UNP O14737
A	3	SER	-	cloning artifact	UNP O14737
A	4	GLY	-	cloning artifact	UNP O14737
A	5	SER	-	cloning artifact	UNP O14737
A	6	SER	-	cloning artifact	UNP O14737
A	7	GLY	-	cloning artifact	UNP O14737
A	113	SER	-	cloning artifact	UNP O14737
A	114	GLY	-	cloning artifact	UNP O14737
A	115	PRO	-	cloning artifact	UNP O14737
A	116	SER	-	cloning artifact	UNP O14737
A	117	SER	-	cloning artifact	UNP O14737
A	118	GLY	-	cloning artifact	UNP O14737

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: Programmed cell death protein 5

Chain A: 37% 15% 47%

G1 S2 S3 G4 S5 S6 G7 L8 R9 R10 Q11 R12 L13 A14 E15 L16 Q17 A18 K19 H20 G21 D22 P23 G24 D25 A26 A27 Q28 Q29 E30 A31 K32 H33 R34 E35 A36 R39 I42 V46 L47 D48 Q49 R52 K65 T66 V69 E70 L73 S87 E88 L91

I92 E93 I94 L95 V98 S99 Q100 Q101 T102 E103 K104 T105 T106 T107 V108 K109 F110 N111 R112 S113 G114 P115 S116 S117 G118

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: Programmed cell death protein 5

Chain A: 35% 17% • 47%

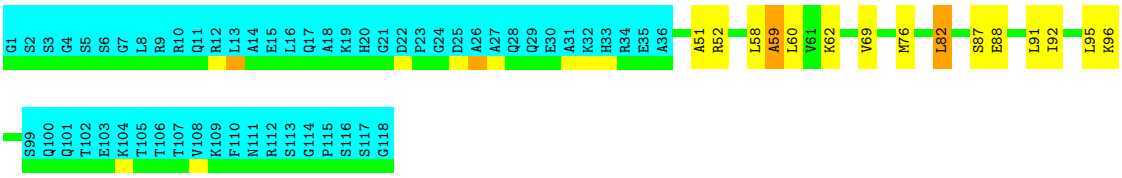
G1 S2 S3 G4 S5 S6 G7 L8 R9 R10 Q11 R12 L13 A14 E15 L16 Q17 A18 K19 H20 G21 D22 P23 G24 D25 A26 A27 Q28 Q29 E30 A31 K32 H33 R34 E35 A36 R39 I42 V46 L47 R54 L55 S56 N57 L58 A59 L60 K65 T66 K67 A68 V69 L73

S87 E88 L91 I94 L95 K96 K97 V98 S99 Q100 Q101 T102 E103 K104 T105 T106 T107 V108 K109 F110 N111 R112 S113 G114 P115 S116 S117 G118

4.2.2 Score per residue for model 2

• Molecule 1: Programmed cell death protein 5

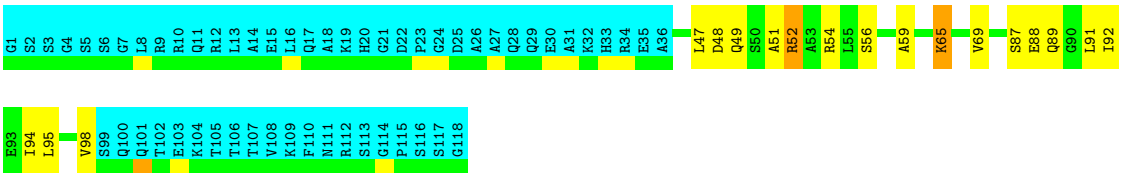
Chain A: 40% 11% • 47%



4.2.3 Score per residue for model 3

- Molecule 1: Programmed cell death protein 5

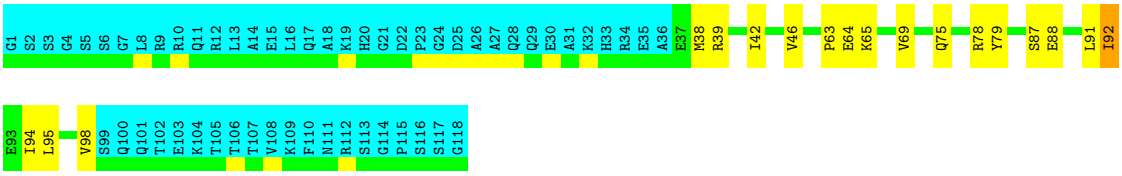
Chain A: 37% 14% • 47%



4.2.4 Score per residue for model 4

- Molecule 1: Programmed cell death protein 5

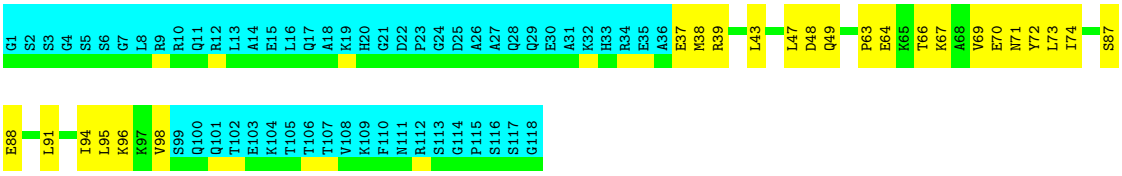
Chain A: 37% 14% • 47%



4.2.5 Score per residue for model 5

- Molecule 1: Programmed cell death protein 5

Chain A: 32% 20% 47%



4.2.6 Score per residue for model 6

- Molecule 1: Programmed cell death protein 5

Chain A: 33% 19% 47%

G1 S2 S3 G4 S5 S6 G7 L8 R9 R10 Q11 R12 L13 A14 E15 L16 Q17 A18 K19 H20 G21 D22 P23 G24 D25 A26 A27 Q28 Q29 E30 A31 K32 H33 R34 E35 A36 E37 M38 I42 L43 V46 A51 R52 P63 E64 V69 E70 N71 Y72 L73 I74 A77 G80

S87 E88 L91 I92 E93 I94 L95 K96 K97 V98 S99 Q100 Q101 T102 E103 K104 T105 T106 T107 V108 K109 F110 N111 R112 S113 G114 P115 S116 S117 G118

4.2.7 Score per residue for model 7

- Molecule 1: Programmed cell death protein 5

Chain A: 43% 8% • 47%

G1 S2 S3 G4 S5 S6 G7 L8 R9 R10 Q11 R12 L13 A14 E15 L16 Q17 A18 K19 H20 G21 D22 P23 G24 D25 A26 A27 Q28 Q29 E30 A31 K32 H33 R34 E35 A36 E37 M38 R39 I42 L58 K65 V69 S87 E88 L95 K96 K97 V98 S99 Q100 Q101 T102 E103

K104 T105 T106 T107 V108 K109 F110 N111 R112 S113 G114 P115 S116 S117 G118

4.2.8 Score per residue for model 8

- Molecule 1: Programmed cell death protein 5

Chain A: 36% 14% • 47%

G1 S2 S3 G4 S5 S6 G7 L8 R9 R10 Q11 R12 L13 A14 E15 L16 Q17 A18 K19 H20 G21 D22 P23 G24 D25 A26 A27 Q28 Q29 E30 A31 K32 H33 R34 E35 A36 V46 L47 D48 Q49 S50 A51 R52 V61 K62 V69 E70 N71 Y72 L73 I74 Q75 M76 A77 Q89 G90

L91 I92 E93 I94 L95 S99 Q100 Q101 T102 E103 K104 T105 T106 T107 V108 K109 F110 N111 R112 S113 G114 P115 S116 S117 G118

4.2.9 Score per residue for model 9

- Molecule 1: Programmed cell death protein 5

Chain A: 36% 14% • 47%

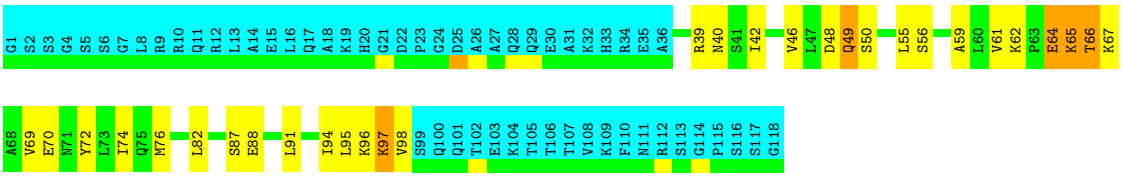
G1 S2 S3 G4 S5 S6 G7 L8 R9 R10 Q11 R12 L13 A14 E15 L16 Q17 A18 K19 H20 G21 D22 P23 G24 D25 A26 A27 Q28 Q29 E30 A31 K32 H33 R34 E35 A36 I42 V46 L47 D48 Q49 S50 A51 R52 V61 K65 T66 K67 A68 V69 E70 L73 M76

L82 S87 E88 I94 L95 V98 S99 Q100 Q101 T102 E103 K104 T105 T106 T107 V108 K109 F110 N111 R112 S113 G114 P115 S116 S117 G118

4.2.10 Score per residue for model 10

- Molecule 1: Programmed cell death protein 5

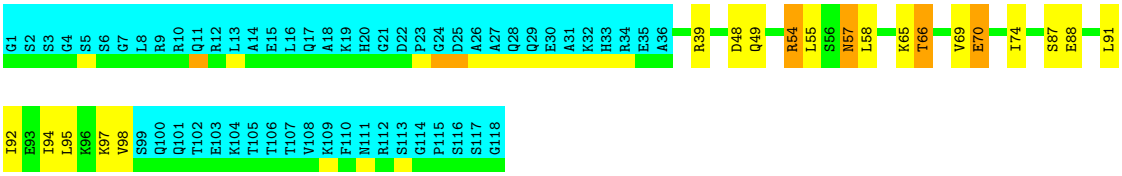
Chain A: 27% 21% • 47%



4.2.11 Score per residue for model 11

- Molecule 1: Programmed cell death protein 5

Chain A: 36% 14% • 47%



4.2.12 Score per residue for model 12

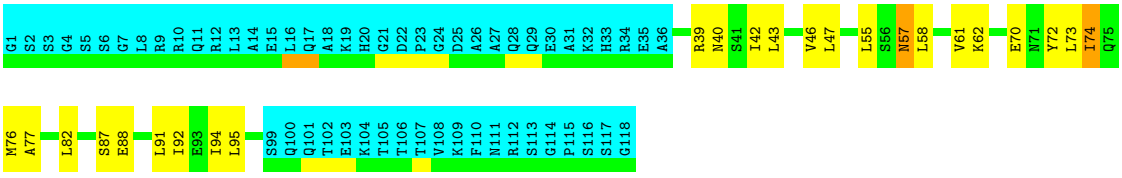
- Molecule 1: Programmed cell death protein 5

Chain A: 28% 24% • 47%

4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Programmed cell death protein 5

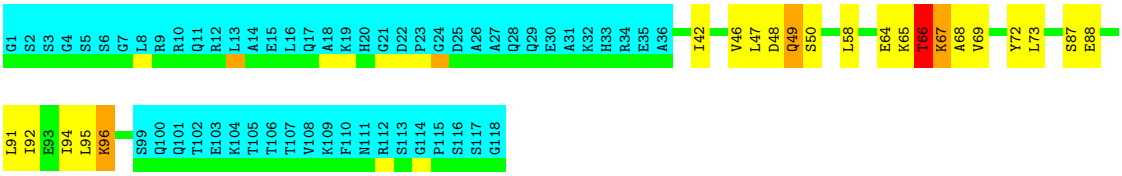
Chain A: 32% 19% • 47%



4.2.14 Score per residue for model 14

- Molecule 1: Programmed cell death protein 5

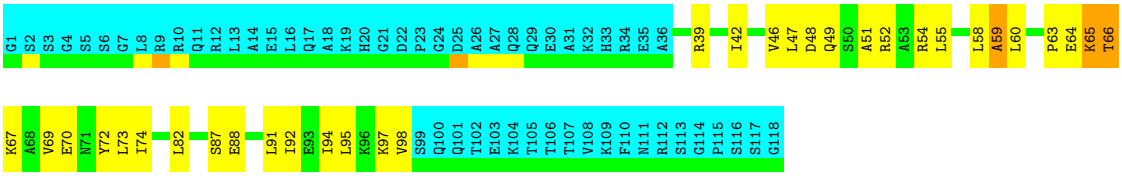
Chain A: 34% 15% • • 47%



4.2.15 Score per residue for model 15

- Molecule 1: Programmed cell death protein 5

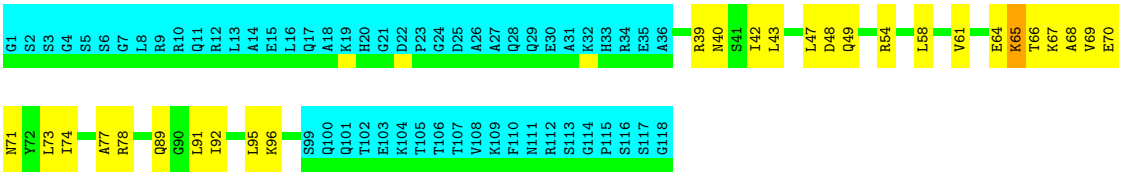
Chain A: 25% 25% • 47%



4.2.16 Score per residue for model 16

- Molecule 1: Programmed cell death protein 5

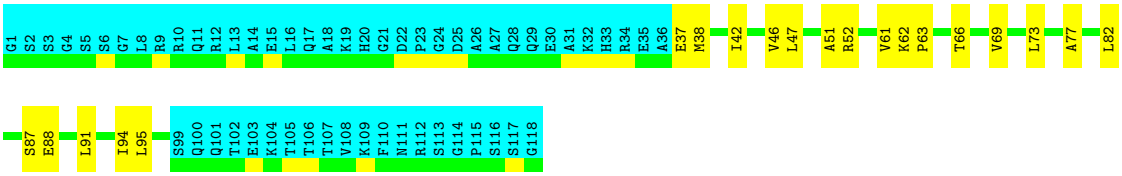
Chain A: 30% 22% • 47%



4.2.17 Score per residue for model 17

- Molecule 1: Programmed cell death protein 5

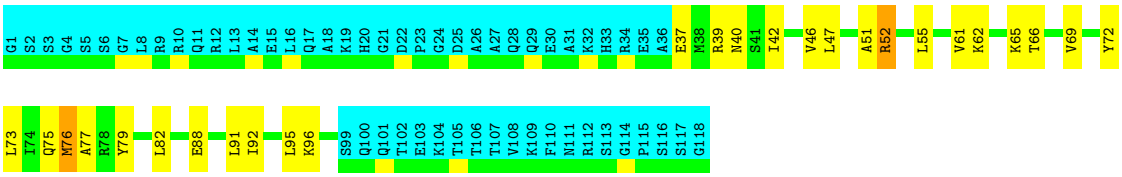
Chain A: 36% 17% 47%



4.2.18 Score per residue for model 18

- Molecule 1: Programmed cell death protein 5

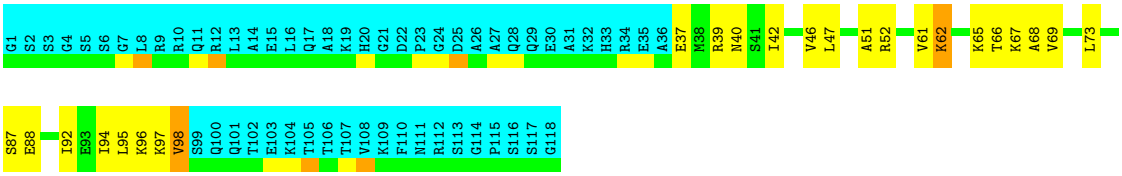
Chain A: 31% 20% • 47%



4.2.19 Score per residue for model 19

- Molecule 1: Programmed cell death protein 5

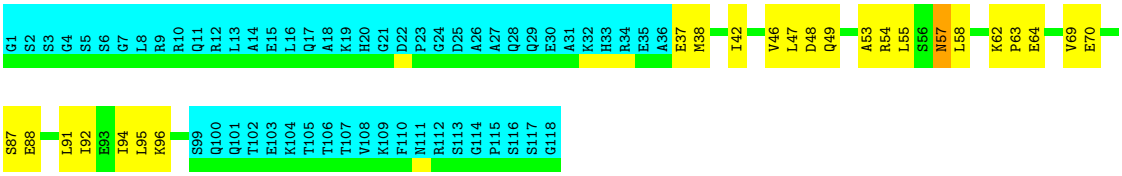
Chain A: 32% 19% • 47%



4.2.20 Score per residue for model 20

- Molecule 1: Programmed cell death protein 5

Chain A: 32% 19% • 47%



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*.

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	490	527	527	16±4
All	All	9800	10540	10540	321

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:VAL:HG21	1:A:95:LEU:HD23	1.05	1.16	12	17
1:A:47:LEU:HD21	1:A:73:LEU:HD13	1.04	1.26	18	4
1:A:69:VAL:HG22	1:A:98:VAL:HG11	0.99	1.31	19	6
1:A:73:LEU:HD21	1:A:94:ILE:HD13	0.82	1.51	5	1
1:A:69:VAL:HG21	1:A:95:LEU:CD2	0.80	2.05	11	13
1:A:72:TYR:CD2	1:A:98:VAL:HG12	0.76	2.15	12	2
1:A:76:MET:SD	1:A:82:LEU:HD21	0.74	2.22	9	2
1:A:69:VAL:CG2	1:A:95:LEU:HD23	0.72	2.06	12	10
1:A:47:LEU:HD21	1:A:73:LEU:CD1	0.70	2.13	1	4
1:A:47:LEU:CD2	1:A:73:LEU:HD13	0.67	2.15	18	2
1:A:55:LEU:HD21	1:A:70:GLU:CG	0.67	2.20	20	1
1:A:92:ILE:HG22	1:A:96:LYS:NZ	0.66	2.04	19	1
1:A:91:LEU:O	1:A:95:LEU:HD12	0.65	1.92	20	2
1:A:42:ILE:O	1:A:46:VAL:HG22	0.64	1.92	1	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:MET:O	1:A:42:ILE:HD12	0.64	1.91	17	4
1:A:69:VAL:HG21	1:A:95:LEU:HD13	0.61	1.70	8	1
1:A:39:ARG:CB	1:A:74:ILE:HD11	0.61	2.25	11	1
1:A:76:MET:HE3	1:A:82:LEU:HD21	0.61	1.72	10	2
1:A:76:MET:CE	1:A:82:LEU:HD21	0.61	2.26	10	3
1:A:43:LEU:HD21	1:A:70:GLU:O	0.60	1.96	5	2
1:A:94:ILE:O	1:A:98:VAL:HG12	0.60	1.97	6	3
1:A:58:LEU:HD11	1:A:62:LYS:NZ	0.59	2.12	20	1
1:A:46:VAL:HG23	1:A:47:LEU:HG	0.59	1.75	18	4
1:A:61:VAL:HG13	1:A:62:LYS:HG2	0.59	1.74	8	1
1:A:73:LEU:HD21	1:A:94:ILE:CD1	0.58	2.27	5	1
1:A:46:VAL:HG11	1:A:77:ALA:HB2	0.57	1.75	8	3
1:A:55:LEU:CD1	1:A:66:THR:HG23	0.56	2.31	1	1
1:A:57:ASN:ND2	1:A:57:ASN:C	0.56	2.59	11	3
1:A:65:LYS:O	1:A:69:VAL:HG23	0.55	2.01	11	2
1:A:72:TYR:CG	1:A:98:VAL:HG12	0.55	2.37	15	1
1:A:39:ARG:HA	1:A:42:ILE:HD12	0.54	1.78	1	4
1:A:72:TYR:CE2	1:A:94:ILE:HG23	0.54	2.37	5	4
1:A:77:ALA:HA	1:A:82:LEU:HD12	0.54	1.78	18	1
1:A:47:LEU:HD21	1:A:73:LEU:HD11	0.53	1.78	19	2
1:A:92:ILE:HA	1:A:95:LEU:HD12	0.53	1.79	12	1
1:A:52:ARG:HH21	1:A:55:LEU:HD23	0.53	1.63	18	1
1:A:58:LEU:HD12	1:A:95:LEU:HD13	0.53	1.80	16	1
1:A:47:LEU:HD11	1:A:73:LEU:CD1	0.52	2.34	15	1
1:A:72:TYR:HE2	1:A:94:ILE:HG23	0.52	1.63	5	2
1:A:61:VAL:HG23	1:A:62:LYS:H	0.52	1.64	10	2
1:A:71:ASN:HA	1:A:74:ILE:HD12	0.51	1.81	16	3
1:A:55:LEU:HD11	1:A:70:GLU:OE1	0.51	2.05	11	1
1:A:65:LYS:HE2	1:A:98:VAL:HG13	0.51	1.82	3	1
1:A:91:LEU:O	1:A:94:ILE:N	0.50	2.43	8	13
1:A:69:VAL:HG21	1:A:95:LEU:CD1	0.50	2.37	8	1
1:A:73:LEU:CD2	1:A:94:ILE:HD13	0.50	2.36	9	1
1:A:94:ILE:O	1:A:97:LYS:N	0.50	2.45	15	2
1:A:42:ILE:O	1:A:46:VAL:HG13	0.50	2.07	4	5
1:A:70:GLU:O	1:A:74:ILE:HD12	0.50	2.06	8	2
1:A:94:ILE:O	1:A:98:VAL:HG13	0.50	2.06	12	1
1:A:56:SER:O	1:A:59:ALA:HB3	0.50	2.06	10	2
1:A:58:LEU:CD1	1:A:95:LEU:HD13	0.49	2.38	16	1
1:A:46:VAL:CG1	1:A:82:LEU:HD13	0.49	2.38	15	1
1:A:61:VAL:HG13	1:A:62:LYS:N	0.49	2.23	19	2
1:A:39:ARG:CG	1:A:40:ASN:N	0.49	2.76	13	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:LEU:HD11	1:A:62:LYS:HZ2	0.49	1.68	20	1
1:A:76:MET:HE1	1:A:82:LEU:HD21	0.49	1.83	13	1
1:A:46:VAL:CG1	1:A:82:LEU:HD22	0.49	2.38	17	1
1:A:69:VAL:O	1:A:72:TYR:N	0.49	2.46	12	3
1:A:72:TYR:CD2	1:A:98:VAL:CG2	0.49	2.96	5	1
1:A:55:LEU:HD21	1:A:70:GLU:OE1	0.48	2.09	15	1
1:A:38:MET:C	1:A:42:ILE:HD12	0.48	2.29	20	1
1:A:58:LEU:HD21	1:A:65:LYS:HG2	0.48	1.86	7	1
1:A:91:LEU:HG	1:A:95:LEU:HD11	0.48	1.86	13	1
1:A:91:LEU:O	1:A:92:ILE:C	0.47	2.53	8	8
1:A:72:TYR:CE2	1:A:76:MET:SD	0.47	3.08	8	1
1:A:76:MET:SD	1:A:82:LEU:HD11	0.47	2.49	9	1
1:A:58:LEU:HD23	1:A:66:THR:OG1	0.46	2.10	1	1
1:A:58:LEU:O	1:A:60:LEU:N	0.46	2.48	2	3
1:A:74:ILE:O	1:A:77:ALA:N	0.46	2.48	13	1
1:A:75:GLN:O	1:A:79:TYR:CD2	0.46	2.68	18	1
1:A:39:ARG:HB2	1:A:74:ILE:HD11	0.46	1.87	11	1
1:A:92:ILE:O	1:A:96:LYS:CD	0.46	2.64	14	1
1:A:48:ASP:O	1:A:50:SER:N	0.46	2.48	14	2
1:A:55:LEU:HD21	1:A:70:GLU:HG2	0.46	1.87	20	1
1:A:61:VAL:HG13	1:A:62:LYS:CG	0.45	2.40	8	1
1:A:54:ARG:O	1:A:57:ASN:N	0.45	2.49	20	1
1:A:87:SER:O	1:A:88:GLU:C	0.45	2.55	13	17
1:A:48:ASP:O	1:A:49:GLN:C	0.45	2.55	3	9
1:A:61:VAL:HG23	1:A:62:LYS:N	0.45	2.27	10	1
1:A:57:ASN:ND2	1:A:58:LEU:N	0.45	2.63	20	3
1:A:66:THR:O	1:A:68:ALA:N	0.45	2.50	14	1
1:A:72:TYR:CD2	1:A:76:MET:SD	0.45	3.10	8	1
1:A:66:THR:O	1:A:67:LYS:C	0.45	2.55	9	4
1:A:47:LEU:CD1	1:A:55:LEU:HD22	0.45	2.42	13	1
1:A:65:LYS:NZ	1:A:95:LEU:O	0.45	2.50	1	1
1:A:63:PRO:O	1:A:64:GLU:C	0.45	2.55	5	5
1:A:77:ALA:O	1:A:80:GLY:N	0.45	2.50	6	1
1:A:92:ILE:HG22	1:A:96:LYS:HE3	0.45	1.89	6	1
1:A:41:SER:O	1:A:44:ALA:N	0.45	2.49	12	1
1:A:58:LEU:O	1:A:59:ALA:C	0.44	2.56	12	3
1:A:95:LEU:N	1:A:95:LEU:CD2	0.44	2.80	8	1
1:A:39:ARG:O	1:A:40:ASN:C	0.44	2.55	19	1
1:A:65:LYS:O	1:A:68:ALA:HB3	0.44	2.11	14	1
1:A:51:ALA:O	1:A:52:ARG:C	0.44	2.56	15	9
1:A:72:TYR:O	1:A:75:GLN:CG	0.44	2.65	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:VAL:O	1:A:70:GLU:C	0.44	2.55	6	2
1:A:64:GLU:O	1:A:65:LYS:C	0.44	2.55	10	1
1:A:97:LYS:CG	1:A:98:VAL:N	0.44	2.81	10	1
1:A:66:THR:O	1:A:69:VAL:N	0.44	2.50	14	1
1:A:95:LEU:HD12	1:A:95:LEU:H	0.44	1.72	20	1
1:A:88:GLU:OE2	1:A:92:ILE:HD11	0.44	2.12	13	2
1:A:39:ARG:HG3	1:A:40:ASN:N	0.43	2.28	10	3
1:A:51:ALA:O	1:A:54:ARG:N	0.43	2.52	15	1
1:A:63:PRO:O	1:A:66:THR:N	0.43	2.52	17	1
1:A:56:SER:O	1:A:59:ALA:CB	0.43	2.66	3	1
1:A:58:LEU:O	1:A:61:VAL:N	0.43	2.52	12	1
1:A:67:LYS:O	1:A:68:ALA:C	0.43	2.56	16	2
1:A:47:LEU:CD2	1:A:91:LEU:HD13	0.43	2.43	3	2
1:A:65:LYS:O	1:A:66:THR:C	0.43	2.57	15	1
1:A:92:ILE:HG22	1:A:96:LYS:HZ2	0.43	1.70	19	1
1:A:47:LEU:HD22	1:A:91:LEU:HD13	0.43	1.90	5	3
1:A:58:LEU:O	1:A:58:LEU:HD23	0.43	2.14	14	1
1:A:55:LEU:O	1:A:58:LEU:N	0.42	2.52	1	1
1:A:66:THR:HG22	1:A:70:GLU:OE2	0.42	2.14	11	1
1:A:73:LEU:O	1:A:74:ILE:C	0.42	2.57	13	4
1:A:64:GLU:CG	1:A:65:LYS:N	0.42	2.82	16	1
1:A:58:LEU:C	1:A:60:LEU:N	0.42	2.73	1	1
1:A:92:ILE:HA	1:A:95:LEU:HD13	0.42	1.89	20	1
1:A:48:ASP:CG	1:A:49:GLN:N	0.42	2.73	5	1
1:A:77:ALA:CA	1:A:82:LEU:HD12	0.42	2.45	18	1
1:A:43:LEU:HA	1:A:46:VAL:HG22	0.42	1.90	6	1
1:A:58:LEU:HD22	1:A:66:THR:HG23	0.42	1.92	14	1
1:A:89:GLN:O	1:A:90:GLY:C	0.42	2.58	8	1
1:A:38:MET:O	1:A:42:ILE:CD1	0.42	2.64	17	1
1:A:38:MET:CG	1:A:39:ARG:N	0.42	2.83	12	1
1:A:55:LEU:O	1:A:56:SER:C	0.41	2.57	10	2
1:A:47:LEU:CD2	1:A:91:LEU:CD1	0.41	2.98	5	1
1:A:94:ILE:HG22	1:A:98:VAL:CG1	0.41	2.46	15	1
1:A:61:VAL:HG13	1:A:62:LYS:H	0.41	1.73	19	1
1:A:53:ALA:O	1:A:54:ARG:C	0.41	2.58	20	1
1:A:61:VAL:HG22	1:A:62:LYS:HG2	0.41	1.92	13	1
1:A:42:ILE:CG2	1:A:77:ALA:CB	0.41	2.99	17	1
1:A:75:GLN:O	1:A:79:TYR:CD1	0.41	2.74	4	1
1:A:70:GLU:O	1:A:74:ILE:CD1	0.41	2.69	8	1
1:A:54:ARG:O	1:A:55:LEU:C	0.41	2.59	20	1
1:A:49:GLN:CD	1:A:49:GLN:C	0.41	2.80	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:ALA:HB1	1:A:91:LEU:HD13	0.41	1.93	12	1
1:A:69:VAL:HG21	1:A:95:LEU:HG	0.41	1.93	20	1
1:A:94:ILE:O	1:A:95:LEU:C	0.40	2.59	12	1
1:A:43:LEU:HD11	1:A:70:GLU:HB3	0.40	1.93	16	1
1:A:38:MET:HG3	1:A:39:ARG:N	0.40	2.32	5	1
1:A:54:ARG:O	1:A:57:ASN:OD1	0.40	2.39	11	1
1:A:77:ALA:O	1:A:78:ARG:C	0.40	2.59	16	1
1:A:66:THR:O	1:A:70:GLU:OE1	0.40	2.40	9	1
1:A:46:VAL:HG12	1:A:82:LEU:HD13	0.40	1.93	15	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	62/118 (53%)	48±3 (77±4%)	14±3 (22±4%)	1±1 (1±2%)	18 66
All	All	1240/2360 (53%)	953 (77%)	273 (22%)	14 (1%)	18 66

All 9 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	59	ALA	3
1	A	92	ILE	2
1	A	49	GLN	2
1	A	64	GLU	2
1	A	82	LEU	1
1	A	89	GLN	1
1	A	74	ILE	1
1	A	66	THR	1
1	A	67	LYS	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	54/97 (56%)	51±2 (95±3%)	3±2 (5±3%)	26	75
All	All	1080/1940 (56%)	1022 (95%)	58 (5%)	26	75

All 18 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	65	LYS	9
1	A	66	THR	8
1	A	96	LYS	7
1	A	97	LYS	5
1	A	54	ARG	4
1	A	62	LYS	3
1	A	57	ASN	3
1	A	67	LYS	2
1	A	52	ARG	2
1	A	89	GLN	2
1	A	39	ARG	2
1	A	61	VAL	2
1	A	70	GLU	2
1	A	76	MET	2
1	A	98	VAL	2
1	A	78	ARG	1
1	A	95	LEU	1
1	A	37	GLU	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