Full wwPDB NMR Structure Validation Report (i)

Feb 26, 2022 – 01:11 PM EST

PDB ID	:	2CRY
Title	:	Solution structure of the fifth ig-like domain of human kin of IRRE like 3
Authors	:	Kurosaki, C.; 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:

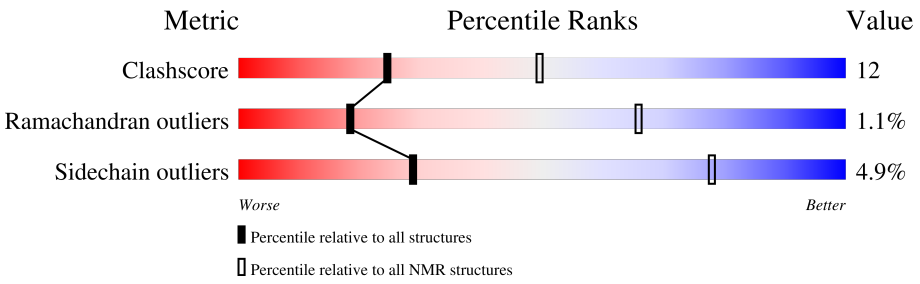
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	122	56% 16% • 28%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 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:13-A:20, A:30-A:109 (88)	0.22	4

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 6 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1806 atoms, of which 889 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Kin of IRRE-like protein 3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	122	1806	565	889	158	191	3	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q8IZU9
A	2	SER	-	cloning artifact	UNP Q8IZU9
A	3	SER	-	cloning artifact	UNP Q8IZU9
A	4	GLY	-	cloning artifact	UNP Q8IZU9
A	5	SER	-	cloning artifact	UNP Q8IZU9
A	6	SER	-	cloning artifact	UNP Q8IZU9
A	7	GLY	-	cloning artifact	UNP Q8IZU9
A	117	SER	-	cloning artifact	UNP Q8IZU9
A	118	GLY	-	cloning artifact	UNP Q8IZU9
A	119	PRO	-	cloning artifact	UNP Q8IZU9
A	120	SER	-	cloning artifact	UNP Q8IZU9
A	121	SER	-	cloning artifact	UNP Q8IZU9
A	122	GLY	-	cloning artifact	UNP Q8IZU9

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: Kin of IRRE-like protein 3

Chain A: 56% 16% • 28%

G1 S2 S3 G4 S5 S6 G7 T8 L9 T10 V11 N12 T20 Q21 T22 Q23 H24 A25 L26 H27 G28 E29 Q32 C35 F36 I37 W48 S49 W50 N53 V54 L55 G61 R62 Y63 T64 V65 V74 I75 S76 T77 I80 S81 R85 A86 D87 F88 I91 K110

E111 Q112 G113 S114 E115 M116 S117 G118 P119 S120 S121 G122

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: Kin of IRRE-like protein 3

Chain A: 56% 15% • 28%

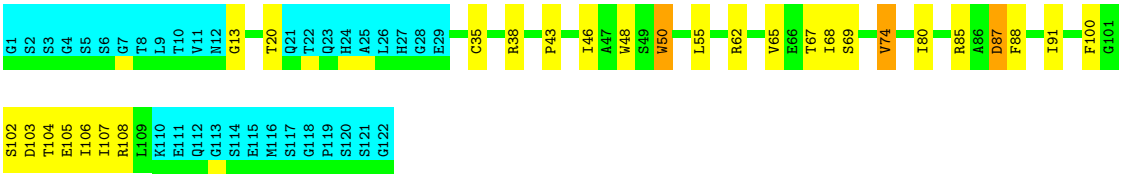
G1 S2 S3 G4 S5 S6 G7 T8 L9 T10 V11 N12 Q21 T22 Q23 H24 A25 L26 H27 G28 E29 Q32 I37 W48 S49 W50 L55 G61 R62 Y63 I68 S69 T70 G73 V74 T77 I80 S81 N82 I83 D87 F88 I91 L109 K110 E111 Q112

G113 S114 E115 M116 S117 G118 P119 S120 S121 G122

4.2.2 Score per residue for model 2

• Molecule 1: Kin of IRRE-like protein 3

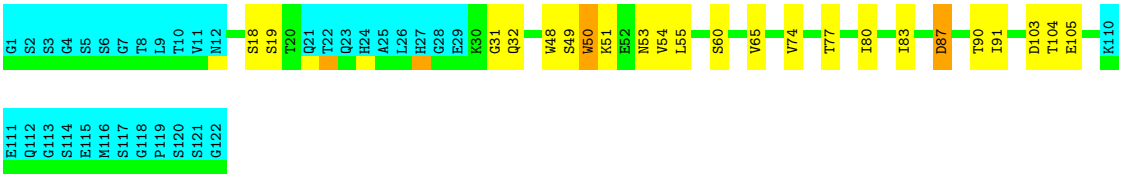
Chain A: 49% 20% • 28%



4.2.3 Score per residue for model 3

- Molecule 1: Kin of IRRE-like protein 3

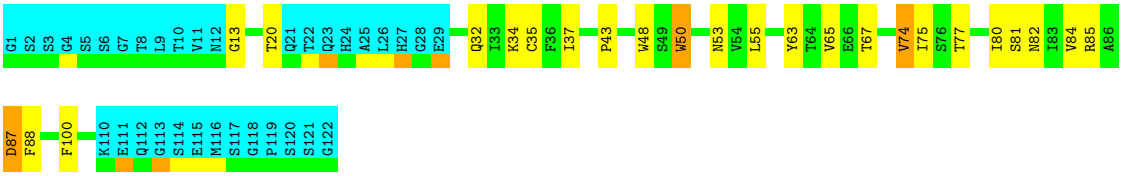
Chain A:



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Kin of IRRE-like protein 3

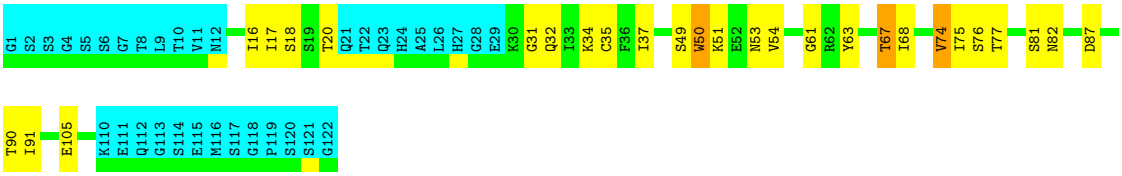
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Kin of IRRE-like protein 3

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Kin of IRRE-like protein 3

Chain A: 48% 22% • 28%

G1 S2 S3 G4 S5 S6 G7 T8 L9 T10 V11 N12 S18 S19 T20 Q21 T22 Q23 H24 A25 L26 H27 G28 E29 K34 C35 F36 P43 W48 S49 W50 K51 E52 N53 V54 L55 E56 S57 G61 R62 Y63 T64 V65 I68 S69 V74 I75 I80 S81 N82 I83 V84

R85 A86 D87 F88 I91 A96 D103 L109 K110 E111 Q112 G113 S114 E115 M116 S117 G118 P119 S120 S121 G122

4.2.7 Score per residue for model 7

- Molecule 1: Kin of IRRE-like protein 3

Chain A: 51% 20% • 28%

G1 S2 S3 G4 S5 S6 G7 T8 L9 T10 V11 N12 G13 T20 Q21 T22 Q23 H24 A25 L26 H27 G28 E29 Q32 C35 F36 I37 R38 S39 W48 S49 W50 K51 E52 L55 T59 Y63 T64 V65 E71 V74 T77 V84 R85 A86 D87 F88 Q89 T90

I91 N98 S99 F100 D103 K110 E111 Q112 G113 S114 E115 M116 S117 G118 P119 S120 S121 G122

4.2.8 Score per residue for model 8

- Molecule 1: Kin of IRRE-like protein 3

Chain A: 48% 22% • 28%

G1 S2 S3 G4 S5 S6 G7 T8 L9 T10 V11 N12 G13 T20 Q21 T22 Q23 H24 A25 L26 H27 G28 E29 Q32 C35 W48 S49 W50 K51 E52 N53 V54 L55 S60 G61 R62 Y63 T64 V65 G73 V74 T77 I80 S81 N82 R85 A86 D87 F88 I91

F100 T104 E105 K110 E111 Q112 G113 S114 E115 M116 S117 G118 P119 S120 S121 G122

4.2.9 Score per residue for model 9

- Molecule 1: Kin of IRRE-like protein 3

Chain A: 52% 18% • 28%

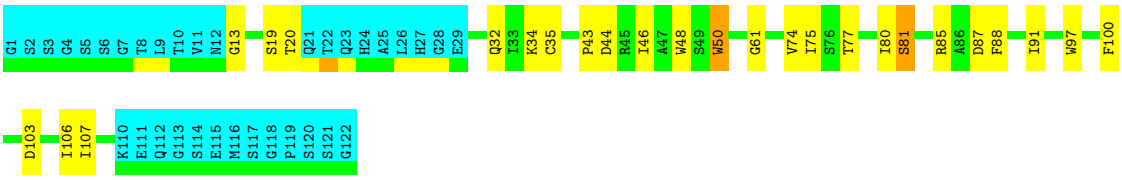
G1 S2 S3 G4 S5 S6 G7 T8 L9 T10 V11 N12 T20 Q21 T22 Q23 H24 A25 L26 H27 G28 E29 I33 K34 C35 P43 W48 S49 W50 K51 L55 R62 Y63 T64 V65 V74 I80 S81 N82 I83 V84 R85 A86 D87 F88 Q89 T90 I91 A96 D103

R108 L109 K110 E111 Q112 G113 S114 E115 M116 S117 G118 P119 S120 S121 G122

4.2.10 Score per residue for model 10

- Molecule 1: Kin of IRRE-like protein 3

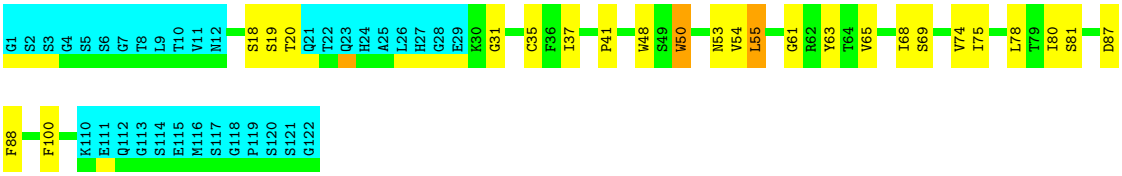
Chain A: 51% 20% • 28%



4.2.11 Score per residue for model 11

- Molecule 1: Kin of IRRE-like protein 3

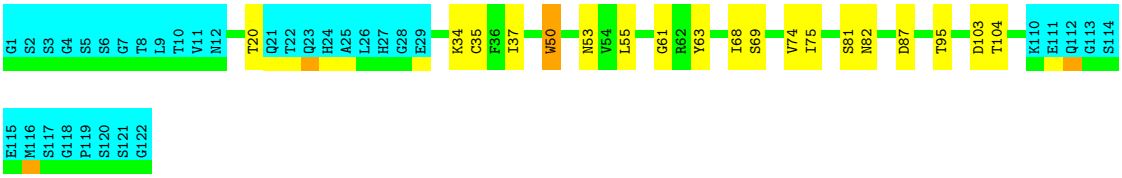
Chain A: 52% 19% • 28%



4.2.12 Score per residue for model 12

- Molecule 1: Kin of IRRE-like protein 3

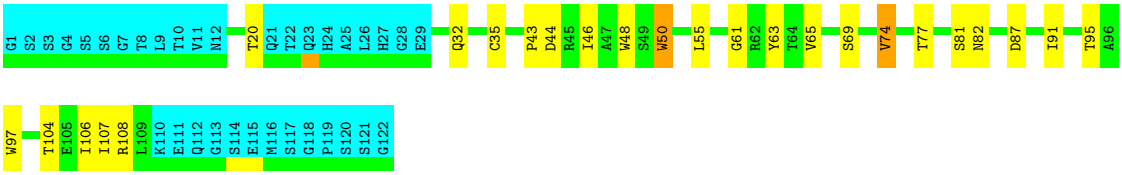
Chain A: 57% 15% • 28%



4.2.13 Score per residue for model 13

- Molecule 1: Kin of IRRE-like protein 3

Chain A: 52% 19% • 28%



4.2.14 Score per residue for model 14

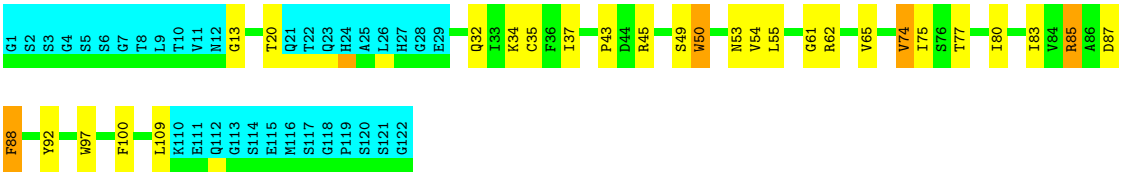
- Molecule 1: Kin of IRRE-like protein 3

Chain A: 52% 19% •• 28%

4.2.15 Score per residue for model 15

- Molecule 1: Kin of IRRE-like protein 3

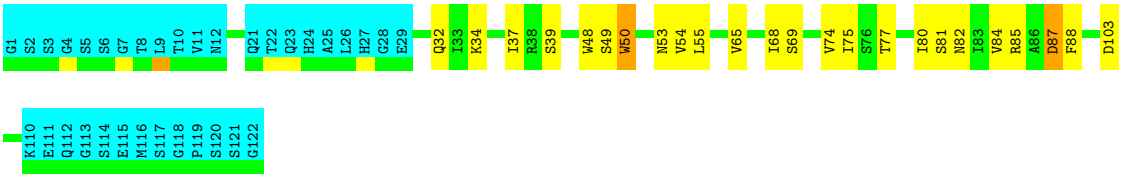
Chain A: 49% 20% • 28%



4.2.16 Score per residue for model 16

- Molecule 1: Kin of IRRE-like protein 3

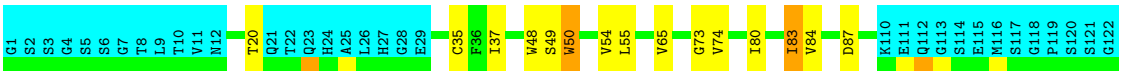
Chain A: 52% 18% • 28%



4.2.17 Score per residue for model 17

- Molecule 1: Kin of IRRE-like protein 3

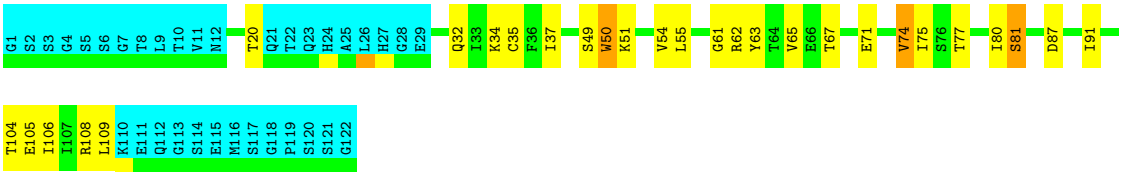
Chain A: 60% 11% • 28%



4.2.18 Score per residue for model 18

- Molecule 1: Kin of IRRE-like protein 3

Chain A: 49% 20% • 28%



4.2.19 Score per residue for model 19

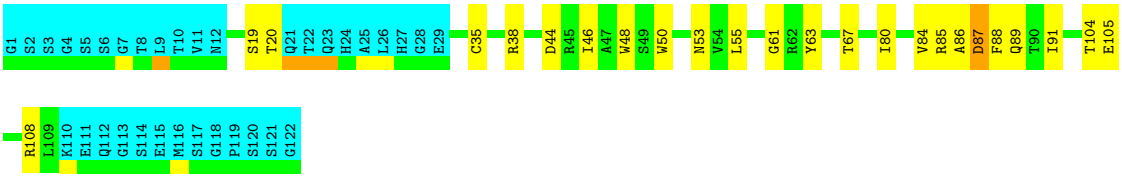
- Molecule 1: Kin of IRRE-like protein 3

Chain A: 52% 19% • 28%

4.2.20 Score per residue for model 20

- Molecule 1: Kin of IRRE-like protein 3

Chain A: 52% 19% • 28%



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	686	678	678	16±3
All	All	13720	13560	13560	322

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:ASP:OD1	1:A:109:LEU:HD23	0.86	1.71	1	2
1:A:55:LEU:HD23	1:A:65:VAL:HG23	0.83	1.50	15	12
1:A:35:CYS:O	1:A:75:ILE:HG23	0.82	1.74	6	5
1:A:37:ILE:HB	1:A:74:VAL:HG23	0.79	1.54	11	11
1:A:96:ALA:HB3	1:A:103:ASP:OD1	0.78	1.77	9	2
1:A:80:ILE:HG21	1:A:87:ASP:OD2	0.76	1.81	2	8
1:A:20:THR:HG22	1:A:35:CYS:HA	0.76	1.56	12	10
1:A:49:SER:HB3	1:A:54:VAL:HG22	0.75	1.57	15	7
1:A:62:ARG:O	1:A:80:ILE:HG23	0.72	1.84	2	3
1:A:49:SER:CB	1:A:54:VAL:HG22	0.71	2.16	18	7
1:A:95:THR:HG23	1:A:104:THR:OG1	0.68	1.88	13	3
1:A:20:THR:HG22	1:A:35:CYS:CA	0.65	2.20	8	6
1:A:80:ILE:HD13	1:A:87:ASP:OD2	0.64	1.92	20	5
1:A:55:LEU:HD13	1:A:65:VAL:HG23	0.63	1.69	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:THR:HG23	1:A:104:THR:HG1	0.63	1.52	13	3
1:A:55:LEU:HD11	1:A:63:TYR:O	0.62	1.95	11	1
1:A:17:ILE:HG22	1:A:105:GLU:OE1	0.61	1.95	5	1
1:A:61:GLY:O	1:A:63:TYR:CD2	0.60	2.54	8	8
1:A:106:ILE:C	1:A:107:ILE:HD12	0.59	2.18	19	4
1:A:51:LYS:HG3	1:A:90:THR:HG23	0.58	1.73	3	2
1:A:20:THR:HG21	1:A:33:ILE:CG2	0.58	2.29	9	1
1:A:87:ASP:OD1	1:A:88:PHE:CD1	0.58	2.57	1	1
1:A:55:LEU:HD22	1:A:65:VAL:CG2	0.58	2.29	17	1
1:A:48:TRP:O	1:A:50:TRP:CZ3	0.56	2.58	7	16
1:A:20:THR:HG22	1:A:35:CYS:HB3	0.56	1.76	13	1
1:A:37:ILE:CB	1:A:74:VAL:HG23	0.56	2.30	11	2
1:A:16:ILE:O	1:A:37:ILE:HG23	0.55	2.02	5	1
1:A:37:ILE:HG22	1:A:39:SER:OG	0.54	2.01	16	1
1:A:88:PHE:CD1	1:A:88:PHE:N	0.54	2.73	15	1
1:A:20:THR:HG22	1:A:35:CYS:CB	0.54	2.33	8	3
1:A:83:ILE:CG2	1:A:84:VAL:N	0.54	2.71	17	2
1:A:43:PRO:HG2	1:A:46:ILE:HD11	0.53	1.81	13	3
1:A:104:THR:HG22	1:A:105:GLU:N	0.53	2.19	8	5
1:A:20:THR:HG22	1:A:35:CYS:SG	0.53	2.43	6	6
1:A:43:PRO:HD2	1:A:74:VAL:HG21	0.52	1.80	4	4
1:A:55:LEU:HD22	1:A:65:VAL:HG23	0.52	1.79	17	1
1:A:91:ILE:CG2	1:A:106:ILE:HG23	0.52	2.34	18	1
1:A:68:ILE:O	1:A:74:VAL:HG12	0.51	2.06	2	1
1:A:83:ILE:HD11	1:A:109:LEU:HD23	0.51	1.83	15	1
1:A:20:THR:CG2	1:A:35:CYS:SG	0.50	3.00	9	4
1:A:67:THR:O	1:A:68:ILE:HD13	0.50	2.06	5	1
1:A:34:LYS:CG	1:A:75:ILE:CG2	0.50	2.90	15	5
1:A:50:TRP:CB	1:A:91:ILE:O	0.50	2.60	3	13
1:A:68:ILE:HG22	1:A:69:SER:H	0.50	1.67	2	2
1:A:13:GLY:C	1:A:100:PHE:CD2	0.50	2.85	10	1
1:A:60:SER:O	1:A:62:ARG:N	0.49	2.44	8	1
1:A:83:ILE:HD11	1:A:87:ASP:CG	0.49	2.28	1	1
1:A:13:GLY:O	1:A:100:PHE:CD2	0.49	2.66	10	2
1:A:32:GLN:CG	1:A:77:THR:CG2	0.49	2.90	14	6
1:A:17:ILE:CG2	1:A:35:CYS:SG	0.49	3.01	5	1
1:A:55:LEU:CD2	1:A:65:VAL:HG23	0.49	2.38	7	2
1:A:44:ASP:N	1:A:97:TRP:O	0.48	2.46	13	2
1:A:37:ILE:CG2	1:A:74:VAL:HG23	0.48	2.38	17	2
1:A:68:ILE:HG22	1:A:69:SER:N	0.48	2.23	16	6
1:A:59:THR:HG23	1:A:63:TYR:O	0.48	2.08	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:GLN:CG	1:A:77:THR:HG22	0.48	2.39	14	1
1:A:61:GLY:O	1:A:63:TYR:CE2	0.47	2.66	8	1
1:A:46:ILE:HD12	1:A:67:THR:HG21	0.47	1.85	20	1
1:A:31:GLY:HA3	1:A:83:ILE:HD12	0.47	1.86	3	1
1:A:13:GLY:HA2	1:A:100:PHE:CD2	0.47	2.45	15	2
1:A:63:TYR:CD1	1:A:80:ILE:HG12	0.47	2.45	9	5
1:A:85:ARG:HA	1:A:88:PHE:CE2	0.47	2.45	15	3
1:A:50:TRP:CA	1:A:91:ILE:O	0.47	2.63	5	4
1:A:18:SER:N	1:A:36:PHE:O	0.47	2.48	6	1
1:A:63:TYR:HB3	1:A:78:LEU:HD11	0.46	1.87	11	1
1:A:13:GLY:HA2	1:A:100:PHE:CD1	0.46	2.45	8	2
1:A:34:LYS:CG	1:A:75:ILE:HG21	0.46	2.40	19	4
1:A:55:LEU:HD21	1:A:63:TYR:O	0.46	2.11	20	2
1:A:80:ILE:O	1:A:81:SER:C	0.45	2.55	1	3
1:A:37:ILE:CG2	1:A:39:SER:OG	0.45	2.65	16	2
1:A:81:SER:O	1:A:82:ASN:C	0.45	2.55	9	8
1:A:41:PRO:HD2	1:A:100:PHE:CE1	0.45	2.46	11	1
1:A:15:PRO:C	1:A:103:ASP:OD2	0.45	2.56	19	1
1:A:32:GLN:HG2	1:A:77:THR:CG2	0.44	2.42	15	9
1:A:103:ASP:OD1	1:A:103:ASP:N	0.44	2.51	9	2
1:A:70:THR:O	1:A:73:GLY:N	0.44	2.50	1	1
1:A:18:SER:OG	1:A:19:SER:N	0.44	2.51	3	1
1:A:85:ARG:HA	1:A:88:PHE:CD2	0.44	2.47	16	5
1:A:50:TRP:CE2	1:A:53:ASN:HB2	0.44	2.47	3	11
1:A:84:VAL:O	1:A:85:ARG:C	0.44	2.56	16	6
1:A:84:VAL:O	1:A:87:ASP:N	0.44	2.51	9	2
1:A:62:ARG:O	1:A:81:SER:N	0.44	2.50	18	1
1:A:96:ALA:CB	1:A:103:ASP:OD1	0.44	2.66	6	1
1:A:102:SER:O	1:A:103:ASP:CG	0.43	2.56	2	1
1:A:34:LYS:HG3	1:A:75:ILE:CG2	0.43	2.43	12	4
1:A:51:LYS:HG2	1:A:90:THR:HG23	0.43	1.89	9	1
1:A:69:SER:HA	1:A:74:VAL:HG12	0.43	1.90	13	1
1:A:87:ASP:CG	1:A:88:PHE:N	0.43	2.71	1	1
1:A:60:SER:OG	1:A:61:GLY:N	0.42	2.53	8	1
1:A:84:VAL:HG23	1:A:86:ALA:HB3	0.42	1.92	19	1
1:A:87:ASP:OD2	1:A:88:PHE:CE1	0.42	2.72	1	1
1:A:55:LEU:CG	1:A:65:VAL:HG23	0.42	2.44	7	1
1:A:53:ASN:O	1:A:54:VAL:CG2	0.41	2.68	11	1
1:A:45:ARG:HG2	1:A:46:ILE:N	0.41	2.30	14	1
1:A:52:GLU:O	1:A:52:GLU:CG	0.41	2.68	7	1
1:A:86:ALA:O	1:A:89:GLN:N	0.41	2.53	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:ASN:O	1:A:100:PHE:N	0.41	2.53	7	1
1:A:55:LEU:HD13	1:A:60:SER:HB3	0.41	1.91	3	1
1:A:35:CYS:SG	1:A:48:TRP:CH2	0.41	3.14	17	1
1:A:16:ILE:O	1:A:37:ILE:CG2	0.41	2.69	5	1
1:A:83:ILE:HD11	1:A:109:LEU:CD2	0.41	2.46	6	2
1:A:55:LEU:HD22	1:A:63:TYR:HB2	0.40	1.91	1	1
1:A:35:CYS:SG	1:A:48:TRP:CZ2	0.40	3.14	17	1
1:A:34:LYS:HG3	1:A:75:ILE:HG21	0.40	1.93	5	2
1:A:83:ILE:HG23	1:A:84:VAL:N	0.40	2.31	17	2
1:A:98:ASN:C	1:A:100:PHE:N	0.40	2.74	7	1
1:A:55:LEU:CD1	1:A:63:TYR:O	0.40	2.68	11	1
1:A:45:ARG:HD2	1:A:97:TRP:CE3	0.40	2.51	15	1
1:A:17:ILE:HG23	1:A:35:CYS:SG	0.40	2.56	5	1
1:A:13:GLY:HA2	1:A:100:PHE:CG	0.40	2.51	10	1
1:A:30:LYS:NZ	1:A:79:THR:HG21	0.40	2.31	14	1
1:A:87:ASP:CG	1:A:92:TYR:OH	0.40	2.60	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	88/122 (72%)	73±2 (83±2%)	14±2 (16±2%)	1±1 (1±1%)	18	66
All	All	1760/2440 (72%)	1465 (83%)	276 (16%)	19 (1%)	18	66

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	61	GLY	6
1	A	81	SER	4
1	A	31	GLY	3
1	A	109	LEU	2
1	A	73	GLY	2
1	A	18	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	83	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	79/105 (75%)	75±2 (95±2%)	4±2 (5±2%)	29 78
All	All	1580/2100 (75%)	1502 (95%)	78 (5%)	29 78

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	50	TRP	18
1	A	87	ASP	15
1	A	74	VAL	12
1	A	103	ASP	5
1	A	67	THR	4
1	A	108	ARG	4
1	A	51	LYS	4
1	A	19	SER	3
1	A	38	ARG	2
1	A	71	GLU	2
1	A	83	ILE	2
1	A	18	SER	1
1	A	76	SER	1
1	A	57	SER	1
1	A	55	LEU	1
1	A	85	ARG	1
1	A	88	PHE	1
1	A	44	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