Full wwPDB NMR Structure Validation Report (i)

Feb 19, 2022 – 03:46 PM EST

PDB ID	:	1RMJ
Title	:	C-terminal domain of insulin-like growth factor (IGF) binding protein-6: structure and interaction with IGF-II
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Deposited on	:	2003-11-28

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:

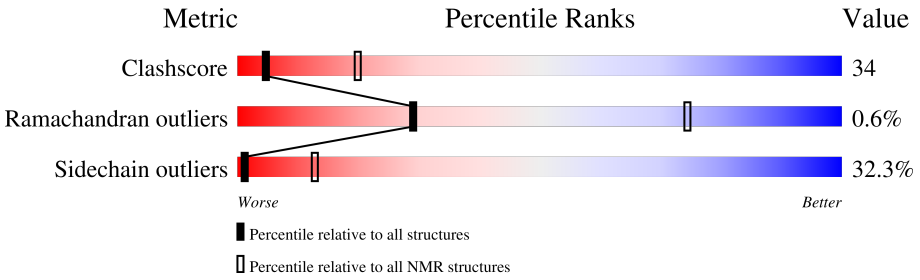
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	107	7% 30% 8% 55%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 20 as representative, based on the following criterion: *closest to the average*.

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:1-A:17, A:24-A:43, A:52-A:62 (48)	0.49	18

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. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1616 atoms, of which 771 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Insulin-like growth factor binding protein 6.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	107	1616	511	771	167	159	8	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	SER	-	cloning artifact	UNP P24592
A	-26	TYR	-	cloning artifact	UNP P24592
A	-25	TYR	-	cloning artifact	UNP P24592
A	-24	HIS	-	cloning artifact	UNP P24592
A	-23	HIS	-	cloning artifact	UNP P24592
A	-22	HIS	-	cloning artifact	UNP P24592
A	-21	HIS	-	cloning artifact	UNP P24592
A	-20	HIS	-	cloning artifact	UNP P24592
A	-19	HIS	-	cloning artifact	UNP P24592
A	-18	ASP	-	cloning artifact	UNP P24592
A	-17	TYR	-	cloning artifact	UNP P24592
A	-16	ASP	-	cloning artifact	UNP P24592
A	-15	ILE	-	cloning artifact	UNP P24592
A	-14	PRO	-	cloning artifact	UNP P24592
A	-13	THR	-	cloning artifact	UNP P24592
A	-12	THR	-	cloning artifact	UNP P24592
A	-11	GLU	-	cloning artifact	UNP P24592
A	-10	ASN	-	cloning artifact	UNP P24592
A	-9	LEU	-	cloning artifact	UNP P24592
A	-8	TYR	-	cloning artifact	UNP P24592
A	-7	PHE	-	cloning artifact	UNP P24592
A	-6	GLN	-	cloning artifact	UNP P24592
A	-5	GLY	-	cloning artifact	UNP P24592
A	-4	ALA	-	cloning artifact	UNP P24592
A	-3	MET	-	cloning artifact	UNP P24592
A	-2	GLY	-	cloning artifact	UNP P24592
A	-1	SER	-	cloning artifact	UNP P24592

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: Insulin-like growth factor binding protein 6

Chain A: 7% 30% 8% 55%

S-27 Y-26 Y-25 H-24 H-23 H-22 H-21 H-20 H-19 D-18 Y-17 D-16 I-15 P-14 T-13 T-12 E-11 N-10 L-9 Y-8 F-7 Q-6 G-5 A-4 M-3 G-2 S-1 C3 R4 R5 H6 L7 D8 S9 V10 L11 Q12 Q13 L14 Q15 T16 E17 V18 Y19 R20 G21 A22 Q23 T24 L25 Y26 V27 P28 N29 C30 D31 H32 R33 G34

F35 Y36 R37 K38 R39 Q40 C41 R42 S43 S44 Q45 G46 Q47 R48 R49 G50 P51 C52 W53 C54 V55 D56 R57 M58 G59 K60 S61 L62 P63 G64 S65 P66 D67 G68 N69 G70 S71 S72 S73 C74 P75 T76 G77 S78 S79 G80

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: Insulin-like growth factor binding protein 6

Chain A: 10% 20% 10% 5% 55%

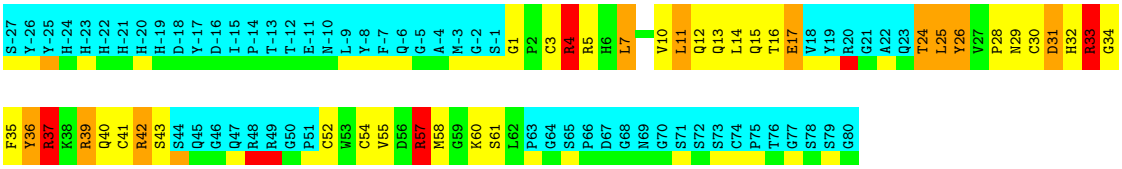
S-27 Y-26 Y-25 H-24 H-23 H-22 H-21 H-20 H-19 D-18 Y-17 D-16 I-15 P-14 T-13 T-12 E-11 N-10 L-9 Y-8 F-7 Q-6 G-5 A-4 M-3 G-2 S-1 G1 P2 C3 R4 R5 H6 L7 D8 S9 V10 L11 Q12 Q13 L14 Q15 V18 Y19 R20 G21 A22 Q23 T24 L25 Y26 N29 C30 D31 H32 R33 G34 F35

Y36 R37 K38 R39 Q40 C41 R42 S43 S44 Q45 G46 Q47 R48 R49 C50 P51 C52 W53 C54 V55 D56 R57 M58 G59 K60 S61 L62 P63 G64 S65 P66 D67 G68 N69 G70 S71 S72 S73 C74 P75 T76 G77 S78 S79 G80

4.2.2 Score per residue for model 2

• Molecule 1: Insulin-like growth factor binding protein 6

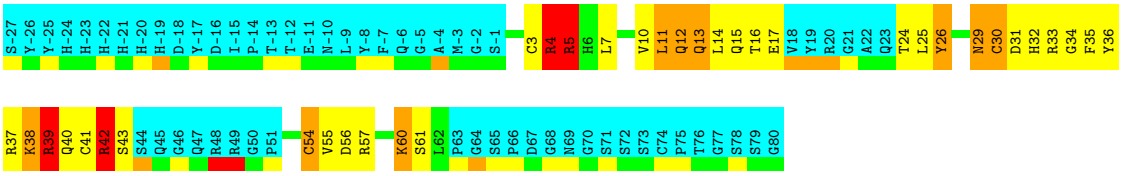
Chain A: 9% 22% 9% • 55%



4.2.3 Score per residue for model 3

- Molecule 1: Insulin-like growth factor binding protein 6

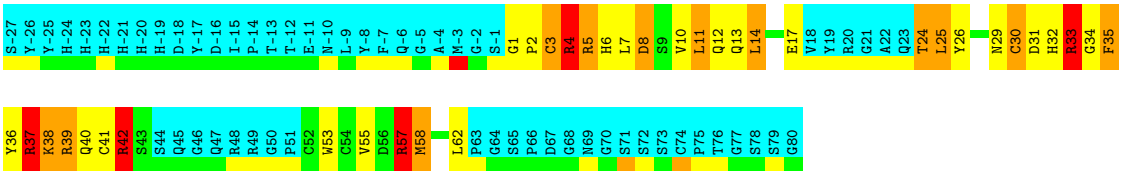
Chain A: 11% 21% 8% • 55%



4.2.4 Score per residue for model 4

- Molecule 1: Insulin-like growth factor binding protein 6

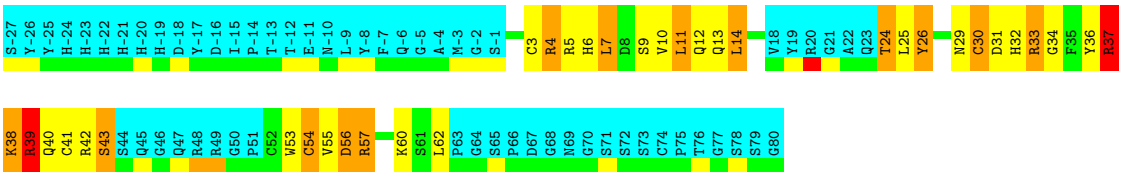
Chain A: 11% 18% 11% 5% 55%



4.2.5 Score per residue for model 5

- Molecule 1: Insulin-like growth factor binding protein 6

Chain A: 12% 19% 12% • 55%



4.2.6 Score per residue for model 6

- Molecule 1: Insulin-like growth factor binding protein 6

Chain A: 9% 24% 8% • 55%

S-27 Y-26 Y-25 H-24 H-23 H-22 H-21 H-20 H-19 D-18 Y-17 D-16 I-15 P-14 T-13 T-12 E-11 N-10 L-9 Y-8 F-7 Q-6 G-5 A-4 M-3 G-2 S-1 G1 P2 C3 R4 R5 H6 L7 D8 S9 V10 Q13 L14 E17 V18 Y19 R20 G21 A22 Q23 T24 L25 Y26 V27 P28 N29 C30 D31 H32 R33 G34 F35

Y36 R37 K38 R39 Q40 C41 R42 S43 S44 Q45 G46 Q47 R48 R49 G50 P51 C52 W53 C54 V55 D56 R57 M58 G59 K60 S61 L62 P63 G64 S65 P66 D67 G68 N69 G70 S71 S72 S73 C74 P75 T76 G77 S78 S79 G80

4.2.7 Score per residue for model 7

- Molecule 1: Insulin-like growth factor binding protein 6

Chain A: 11% 23% 8% • 55%

S-27 Y-26 Y-25 H-24 H-23 H-22 H-21 H-20 H-19 D-18 Y-17 D-16 I-15 P-14 T-13 T-12 E-11 N-10 L-9 Y-8 F-7 Q-6 G-5 A-4 M-3 G-2 S-1 C3 R4 R5 H6 L11 Q12 Q13 L14 Q15 T16 E17 V18 Y19 R20 G21 A22 Q23 T24 L25 Y26 V27 P28 N29 C30 D31 H32 R33 G34 F35 Y36 R37

K38 R39 Q40 C41 R42 S43 S44 Q45 G46 Q47 R48 R49 G50 P51 C52 W53 C54 V55 D56 R57 M58 G59 K60 S61 L62 P63 G64 S65 P66 D67 G68 N69 G70 S71 S72 S73 C74 P75 T76 G77 S78 S79 G80

4.2.8 Score per residue for model 8

- Molecule 1: Insulin-like growth factor binding protein 6

Chain A: 10% 23% 9% • 55%

S-27 Y-26 Y-25 H-24 H-23 H-22 H-21 H-20 H-19 D-18 Y-17 D-16 I-15 P-14 T-13 T-12 E-11 N-10 L-9 Y-8 F-7 Q-6 G-5 A-4 M-3 G-2 S-1 G1 P2 C3 R4 R5 H6 L7 D8 S9 V10 L11 L14 Q15 T16 E17 V18 Y19 R20 G21 A22 Q23 T24 L25 Y26 V27 P28 N29 C30 D31 H32 R33 G34

F35 Y36 R37 K38 R39 Q40 C41 R42 S43 S44 Q45 G46 Q47 R48 R49 G50 P51 C52 W53 C54 V55 D56 R57 M58 G59 K60 S61 L62 P63 G64 S65 P66 D67 G68 N69 G70 S71 S72 S73 C74 P75 T76 G77 S78 S79 G80

4.2.9 Score per residue for model 9

- Molecule 1: Insulin-like growth factor binding protein 6

Chain A: 10% 22% 10% • 55%

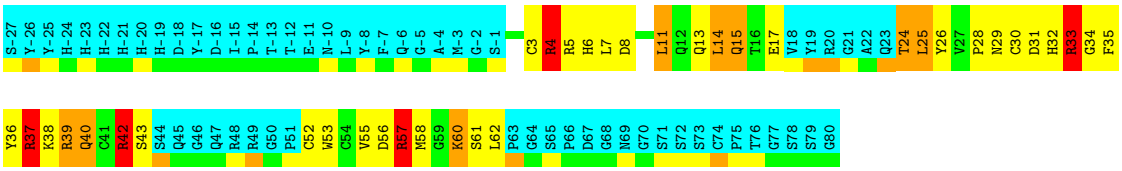
S-27 Y-26 Y-25 H-24 H-23 H-22 H-21 H-20 H-19 D-18 Y-17 D-16 I-15 P-14 T-13 T-12 E-11 N-10 L-9 Y-8 F-7 Q-6 G-5 A-4 M-3 G-2 S-1 C3 R4 R5 H6 L7 D8 S9 V10 L11 Q12 Q13 L14 Q15 T16 E17 V18 Y19 R20 G21 A22 Q23 T24 L25 Y26 N29 C30 D31 H32 R33 G34 F35

Y36 R37 K38 R39 Q40 C41 R42 S43 S44 Q45 G46 Q47 R48 R49 G50 P51 C52 W53 C54 V55 D56 R57 M58 G59 K60 P63 G64 S65 P66 D67 G68 N69 G70 S71 S72 S73 C74 P75 T76 G77 S78 S79 G80

4.2.10 Score per residue for model 10

- Molecule 1: Insulin-like growth factor binding protein 6

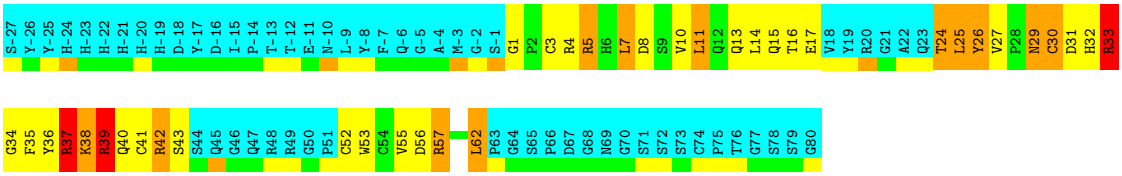
Chain A: 9% 23% 7% 5% 55%



4.2.11 Score per residue for model 11

- Molecule 1: Insulin-like growth factor binding protein 6

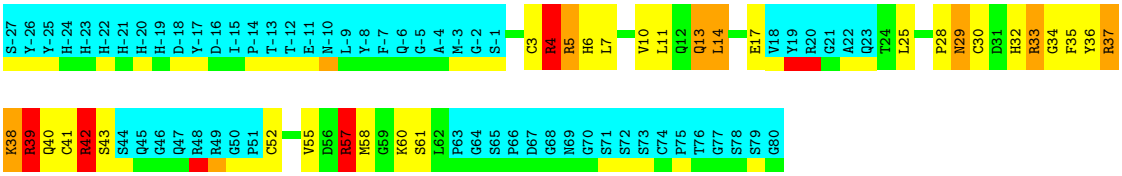
Chain A: 9% 21% 11% • 55%



4.2.12 Score per residue for model 12

- Molecule 1: Insulin-like growth factor binding protein 6

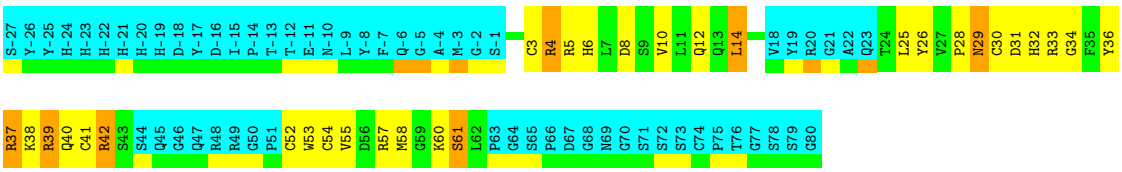
Chain A: 15% 20% 7% • 55%



4.2.13 Score per residue for model 13

- Molecule 1: Insulin-like growth factor binding protein 6

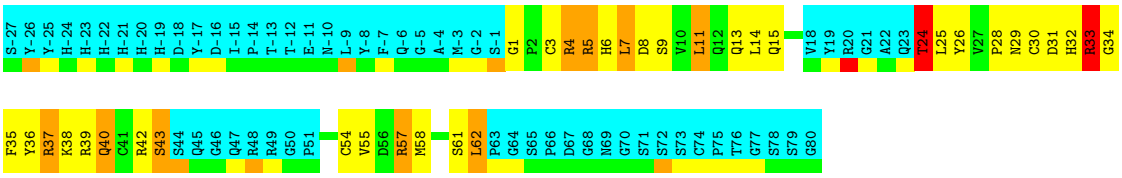
Chain A: 15% 23% 7% 55%



4.2.14 Score per residue for model 14

- Molecule 1: Insulin-like growth factor binding protein 6

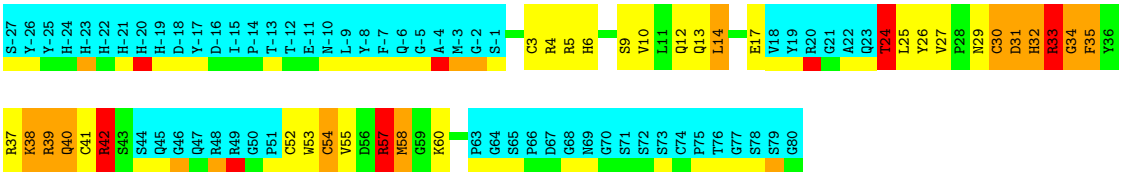
Chain A: 11% 23% 8% • 55%



4.2.15 Score per residue for model 15

- Molecule 1: Insulin-like growth factor binding protein 6

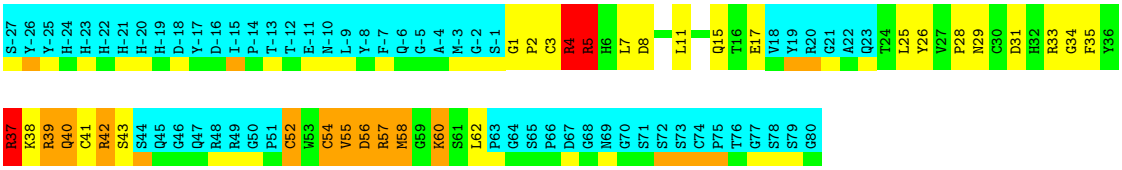
Chain A: 13% 18% 10% • 55%



4.2.16 Score per residue for model 16

- Molecule 1: Insulin-like growth factor binding protein 6

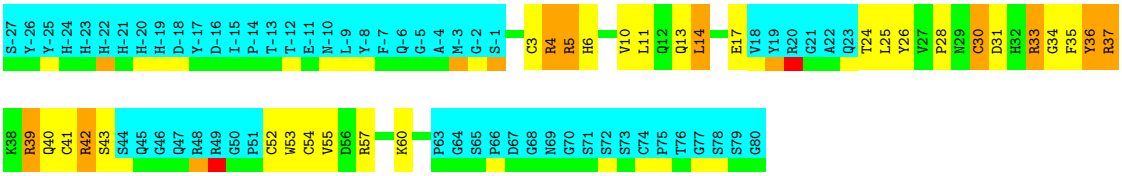
Chain A: 14% 19% 9% • 55%



4.2.17 Score per residue for model 17

- Molecule 1: Insulin-like growth factor binding protein 6

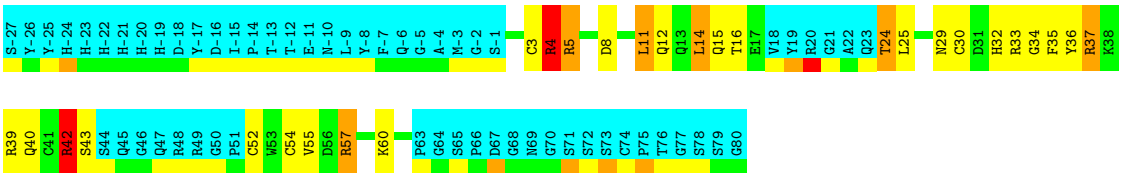
Chain A: 16% 21% 8% 55%



4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Insulin-like growth factor binding protein 6

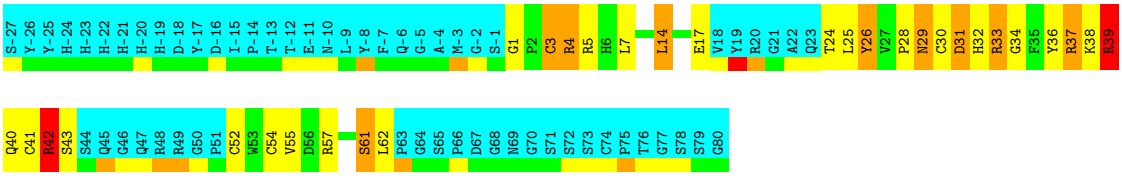
Chain A: 19% 19% 6% • 55%



4.2.19 Score per residue for model 19

- Molecule 1: Insulin-like growth factor binding protein 6

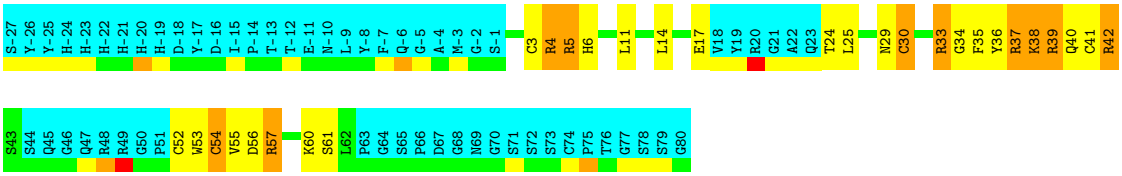
Chain A: 16% 19% 8% • 55%



4.2.20 Score per residue for model 20

- Molecule 1: Insulin-like growth factor binding protein 6

Chain A: 18% 18% 9% 55%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *distance geometry simulated annealing.*

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CYANA	refinement	1.0.3
X-PLOR	structure solution	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.06±0.03	0±0/407 (0.0± 0.1%)	1.31±0.02	0±0/548 (0.0± 0.0%)
All	All	1.06	2/8140 (0.0%)	1.31	1/10960 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	7.0±0.0
All	All	0	140

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	34	GLY	N-CA	6.30	1.55	1.46	15	1
1	A	33	ARG	N-CA	5.56	1.57	1.46	15	1

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	30	CYS	N-CA-CB	-5.21	101.22	110.60	15	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	4	ARG	Sidechain	20

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	5	ARG	Sidechain	20
1	A	33	ARG	Sidechain	20
1	A	37	ARG	Sidechain	20
1	A	39	ARG	Sidechain	20
1	A	42	ARG	Sidechain	20
1	A	57	ARG	Sidechain	20

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	398	387	387	27±7
All	All	7960	7740	7740	533

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 34.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:LEU:HA	1:A:14:LEU:HD23	0.89	1.44	8	6
1:A:40:GLN:CG	1:A:55:VAL:HG11	0.87	1.99	20	12
1:A:40:GLN:HG3	1:A:55:VAL:HG11	0.84	1.47	2	17
1:A:10:VAL:HG13	1:A:14:LEU:HD12	0.84	1.49	2	4
1:A:7:LEU:HD12	1:A:30:CYS:SG	0.81	2.16	14	9
1:A:40:GLN:HG2	1:A:55:VAL:HG11	0.79	1.55	10	1
1:A:3:CYS:SG	1:A:36:TYR:CD1	0.77	2.77	20	4
1:A:3:CYS:SG	1:A:36:TYR:CD2	0.75	2.78	3	8
1:A:39:ARG:HG3	1:A:41:CYS:SG	0.75	2.21	19	2
1:A:40:GLN:HG2	1:A:55:VAL:HG21	0.75	1.57	17	7
1:A:40:GLN:OE1	1:A:55:VAL:HG21	0.75	1.80	10	1
1:A:39:ARG:CD	1:A:52:CYS:SG	0.74	2.76	20	3
1:A:14:LEU:HA	1:A:25:LEU:HD23	0.74	1.59	19	1
1:A:40:GLN:CG	1:A:55:VAL:HG21	0.72	2.13	17	6
1:A:37:ARG:HG2	1:A:38:LYS:N	0.70	2.00	16	1
1:A:39:ARG:CG	1:A:41:CYS:SG	0.70	2.80	5	7
1:A:39:ARG:CD	1:A:41:CYS:SG	0.69	2.80	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ARG:HD3	1:A:41:CYS:SG	0.68	2.28	3	6
1:A:39:ARG:HD2	1:A:41:CYS:SG	0.67	2.30	4	5
1:A:40:GLN:HG3	1:A:55:VAL:HG21	0.67	1.65	9	6
1:A:24:THR:HA	1:A:43:SER:O	0.66	1.90	3	8
1:A:16:THR:HG22	1:A:17:GLU:HG2	0.65	1.68	2	1
1:A:7:LEU:CD2	1:A:11:LEU:HD13	0.65	2.21	8	1
1:A:24:THR:HG22	1:A:42:ARG:HB3	0.65	1.68	2	2
1:A:10:VAL:CG1	1:A:27:VAL:HG12	0.65	2.21	8	1
1:A:54:CYS:SG	1:A:62:LEU:HD12	0.64	2.33	6	2
1:A:31:ASP:HB3	1:A:37:ARG:HB2	0.63	1.70	8	4
1:A:33:ARG:HD3	1:A:35:PHE:HB2	0.63	1.69	4	2
1:A:3:CYS:SG	1:A:28:PRO:HB2	0.63	2.33	14	8
1:A:40:GLN:CB	1:A:55:VAL:HG11	0.62	2.24	16	4
1:A:55:VAL:HG12	1:A:61:SER:HA	0.62	1.70	1	6
1:A:38:LYS:HG2	1:A:39:ARG:N	0.62	2.09	20	1
1:A:10:VAL:O	1:A:14:LEU:HB2	0.62	1.95	1	10
1:A:8:ASP:HA	1:A:11:LEU:HD23	0.61	1.71	4	1
1:A:39:ARG:HG2	1:A:41:CYS:SG	0.61	2.35	8	5
1:A:40:GLN:HB2	1:A:55:VAL:HG11	0.61	1.70	17	3
1:A:14:LEU:HA	1:A:25:LEU:HD21	0.61	1.71	6	1
1:A:14:LEU:HA	1:A:25:LEU:CD2	0.61	2.25	12	2
1:A:26:TYR:HA	1:A:41:CYS:O	0.60	1.96	4	13
1:A:57:ARG:HD3	1:A:58:MET:HG2	0.60	1.71	12	2
1:A:14:LEU:HD12	1:A:15:GLN:N	0.60	2.09	14	1
1:A:31:ASP:HB2	1:A:37:ARG:CB	0.60	2.26	16	3
1:A:31:ASP:HB2	1:A:37:ARG:HB2	0.60	1.74	16	2
1:A:39:ARG:HG2	1:A:40:GLN:N	0.60	2.11	5	3
1:A:29:ASN:CB	1:A:39:ARG:HB3	0.60	2.27	15	6
1:A:3:CYS:HB2	1:A:36:TYR:CD2	0.59	2.31	4	1
1:A:3:CYS:HB3	1:A:34:GLY:O	0.59	1.98	14	15
1:A:4:ARG:N	1:A:30:CYS:SG	0.59	2.76	19	1
1:A:33:ARG:CD	1:A:35:PHE:HB2	0.58	2.28	4	3
1:A:55:VAL:HA	1:A:60:LYS:O	0.58	1.98	16	13
1:A:39:ARG:HD3	1:A:52:CYS:SG	0.58	2.39	12	2
1:A:31:ASP:HB2	1:A:37:ARG:HB3	0.58	1.73	2	2
1:A:14:LEU:HD22	1:A:25:LEU:HD13	0.58	1.74	3	1
1:A:14:LEU:HA	1:A:25:LEU:HD22	0.57	1.73	17	1
1:A:17:GLU:HB2	1:A:25:LEU:HD21	0.57	1.75	17	1
1:A:30:CYS:SG	1:A:34:GLY:C	0.56	2.83	4	1
1:A:10:VAL:HG11	1:A:27:VAL:HA	0.56	1.77	8	1
1:A:31:ASP:CB	1:A:37:ARG:HB2	0.56	2.29	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ARG:HD2	1:A:52:CYS:SG	0.56	2.40	6	3
1:A:40:GLN:HB2	1:A:53:TRP:CE2	0.56	2.36	8	2
1:A:30:CYS:HA	1:A:35:PHE:O	0.56	2.00	11	12
1:A:17:GLU:O	1:A:25:LEU:HD11	0.56	2.00	17	1
1:A:33:ARG:HD3	1:A:35:PHE:CD1	0.56	2.36	10	1
1:A:7:LEU:HD23	1:A:11:LEU:HD23	0.56	1.78	14	1
1:A:25:LEU:HD12	1:A:26:TYR:N	0.56	2.16	19	1
1:A:3:CYS:SG	1:A:34:GLY:O	0.55	2.65	9	1
1:A:26:TYR:C	1:A:26:TYR:CD1	0.55	2.76	8	1
1:A:11:LEU:HA	1:A:15:GLN:HG3	0.55	1.78	11	1
1:A:37:ARG:HA	1:A:57:ARG:HA	0.55	1.79	10	5
1:A:57:ARG:HD2	1:A:58:MET:N	0.55	2.17	15	1
1:A:31:ASP:CB	1:A:37:ARG:HD3	0.55	2.31	4	3
1:A:31:ASP:HB3	1:A:37:ARG:HD2	0.55	1.77	8	1
1:A:14:LEU:C	1:A:14:LEU:HD12	0.54	2.23	18	5
1:A:30:CYS:SG	1:A:34:GLY:O	0.54	2.66	4	1
1:A:11:LEU:HA	1:A:14:LEU:CD2	0.54	2.33	10	4
1:A:31:ASP:CB	1:A:37:ARG:HD2	0.53	2.33	17	3
1:A:31:ASP:HB2	1:A:37:ARG:CD	0.53	2.34	13	1
1:A:3:CYS:CB	1:A:35:PHE:O	0.53	2.57	15	1
1:A:30:CYS:SG	1:A:35:PHE:O	0.52	2.67	15	1
1:A:26:TYR:OH	1:A:40:GLN:HB3	0.52	2.04	17	1
1:A:29:ASN:O	1:A:36:TYR:HA	0.52	2.05	19	7
1:A:33:ARG:HD2	1:A:35:PHE:HB2	0.52	1.80	10	3
1:A:3:CYS:HB2	1:A:36:TYR:CE2	0.52	2.40	4	1
1:A:11:LEU:HD12	1:A:11:LEU:C	0.51	2.24	3	5
1:A:26:TYR:CE2	1:A:28:PRO:HB3	0.51	2.41	14	1
1:A:6:HIS:CD2	1:A:28:PRO:HG3	0.51	2.39	12	1
1:A:36:TYR:HB3	1:A:40:GLN:NE2	0.51	2.21	12	2
1:A:14:LEU:HD12	1:A:14:LEU:C	0.51	2.25	14	1
1:A:10:VAL:HG21	1:A:28:PRO:HD3	0.51	1.80	6	1
1:A:7:LEU:O	1:A:11:LEU:HB2	0.51	2.05	8	2
1:A:38:LYS:HD3	1:A:39:ARG:HG3	0.51	1.82	16	1
1:A:7:LEU:HG	1:A:28:PRO:HG2	0.51	1.82	19	1
1:A:33:ARG:O	1:A:33:ARG:HD3	0.51	2.05	1	1
1:A:26:TYR:CE2	1:A:53:TRP:CZ2	0.51	2.99	17	1
1:A:31:ASP:HB2	1:A:37:ARG:HD2	0.50	1.81	16	1
1:A:38:LYS:O	1:A:55:VAL:N	0.50	2.44	15	3
1:A:10:VAL:HG12	1:A:27:VAL:HG12	0.50	1.83	8	1
1:A:10:VAL:O	1:A:14:LEU:N	0.50	2.42	12	5
1:A:35:PHE:CE1	1:A:58:MET:HE3	0.50	2.42	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:GLN:HG2	1:A:17:GLU:HG3	0.50	1.83	6	1
1:A:10:VAL:HG13	1:A:14:LEU:CD1	0.50	2.34	11	1
1:A:40:GLN:HG2	1:A:55:VAL:CG2	0.50	2.37	18	3
1:A:25:LEU:HD12	1:A:27:VAL:HG23	0.49	1.83	7	1
1:A:29:ASN:HB3	1:A:39:ARG:O	0.49	2.08	9	2
1:A:8:ASP:HA	1:A:11:LEU:CD2	0.49	2.37	18	2
1:A:57:ARG:HD3	1:A:58:MET:N	0.49	2.22	12	1
1:A:29:ASN:HB2	1:A:39:ARG:HD2	0.49	1.83	2	2
1:A:29:ASN:HB2	1:A:39:ARG:HB3	0.49	1.84	7	3
1:A:24:THR:CA	1:A:43:SER:O	0.49	2.61	3	3
1:A:38:LYS:O	1:A:54:CYS:HA	0.49	2.07	5	2
1:A:5:ARG:CZ	1:A:5:ARG:HB3	0.49	2.38	1	1
1:A:6:HIS:O	1:A:10:VAL:HG23	0.48	2.08	4	7
1:A:11:LEU:HG	1:A:12:GLN:N	0.48	2.23	4	3
1:A:28:PRO:HA	1:A:40:GLN:OE1	0.48	2.08	2	1
1:A:29:ASN:ND2	1:A:39:ARG:O	0.48	2.46	19	1
1:A:39:ARG:HG2	1:A:52:CYS:SG	0.48	2.49	20	1
1:A:9:SER:O	1:A:12:GLN:HG2	0.48	2.09	15	2
1:A:56:ASP:CB	1:A:62:LEU:HD11	0.48	2.38	16	1
1:A:39:ARG:CG	1:A:52:CYS:SG	0.48	3.01	20	1
1:A:24:THR:HG22	1:A:24:THR:O	0.48	2.08	2	1
1:A:12:GLN:O	1:A:15:GLN:HG2	0.48	2.09	7	1
1:A:26:TYR:CA	1:A:41:CYS:O	0.47	2.62	2	4
1:A:40:GLN:HB3	1:A:53:TRP:CZ2	0.47	2.43	8	4
1:A:32:HIS:CE1	1:A:33:ARG:HD2	0.47	2.44	14	2
1:A:29:ASN:CB	1:A:39:ARG:O	0.47	2.63	10	2
1:A:11:LEU:O	1:A:15:GLN:HB3	0.47	2.10	3	1
1:A:11:LEU:HA	1:A:15:GLN:HB2	0.47	1.86	1	2
1:A:24:THR:OG1	1:A:42:ARG:NH1	0.47	2.44	8	1
1:A:40:GLN:HB3	1:A:53:TRP:CE2	0.47	2.45	10	1
1:A:26:TYR:CB	1:A:42:ARG:HA	0.47	2.40	2	1
1:A:29:ASN:HB3	1:A:39:ARG:HG2	0.47	1.86	19	1
1:A:4:ARG:HG3	1:A:5:ARG:N	0.46	2.25	3	2
1:A:42:ARG:O	1:A:42:ARG:HG3	0.46	2.11	6	1
1:A:3:CYS:SG	1:A:35:PHE:C	0.46	2.93	9	1
1:A:12:GLN:CG	1:A:13:GLN:N	0.46	2.79	3	4
1:A:31:ASP:HB3	1:A:37:ARG:CB	0.46	2.39	8	2
1:A:39:ARG:HD2	1:A:52:CYS:HB3	0.46	1.87	10	1
1:A:29:ASN:C	1:A:30:CYS:SG	0.46	2.93	15	1
1:A:4:ARG:HD3	1:A:4:ARG:C	0.46	2.30	4	2
1:A:25:LEU:O	1:A:43:SER:N	0.46	2.48	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:CYS:HB2	1:A:36:TYR:CD1	0.46	2.46	14	1
1:A:7:LEU:O	1:A:11:LEU:N	0.46	2.41	3	2
1:A:40:GLN:N	1:A:55:VAL:HG11	0.46	2.26	16	1
1:A:26:TYR:CE2	1:A:53:TRP:CH2	0.46	3.04	17	1
1:A:40:GLN:HG3	1:A:55:VAL:CG1	0.46	2.38	17	2
1:A:41:CYS:CB	1:A:52:CYS:HA	0.45	2.40	7	1
1:A:1:GLY:N	1:A:2:PRO:CD	0.45	2.79	8	1
1:A:27:VAL:HG12	1:A:39:ARG:NH2	0.45	2.27	11	1
1:A:14:LEU:HG	1:A:15:GLN:N	0.45	2.27	8	1
1:A:13:GLN:O	1:A:17:GLU:N	0.45	2.40	15	1
1:A:41:CYS:HA	1:A:52:CYS:HA	0.45	1.86	19	1
1:A:3:CYS:HA	1:A:36:TYR:CE2	0.45	2.46	10	1
1:A:57:ARG:HG3	1:A:58:MET:HG2	0.45	1.88	8	1
1:A:13:GLN:HB3	1:A:17:GLU:HG3	0.45	1.86	12	1
1:A:57:ARG:CD	1:A:58:MET:HG2	0.45	2.39	12	1
1:A:3:CYS:SG	1:A:29:ASN:O	0.45	2.74	19	1
1:A:1:GLY:HA3	1:A:34:GLY:C	0.45	2.32	4	3
1:A:26:TYR:CA	1:A:42:ARG:HA	0.45	2.41	11	2
1:A:31:ASP:HB2	1:A:37:ARG:HD3	0.45	1.89	9	2
1:A:53:TRP:CD1	1:A:55:VAL:HG12	0.45	2.47	8	1
1:A:39:ARG:HD3	1:A:52:CYS:HB3	0.45	1.89	9	1
1:A:14:LEU:HD22	1:A:25:LEU:CD1	0.45	2.41	3	1
1:A:28:PRO:HA	1:A:40:GLN:NE2	0.45	2.27	10	1
1:A:1:GLY:O	1:A:5:ARG:CD	0.45	2.65	11	1
1:A:29:ASN:HB2	1:A:39:ARG:CD	0.44	2.42	1	1
1:A:31:ASP:HB2	1:A:37:ARG:HG2	0.44	1.89	19	1
1:A:39:ARG:O	1:A:40:GLN:NE2	0.44	2.51	12	1
1:A:17:GLU:CB	1:A:25:LEU:HD21	0.44	2.42	17	1
1:A:11:LEU:O	1:A:15:GLN:CB	0.44	2.66	3	2
1:A:38:LYS:O	1:A:55:VAL:HG22	0.44	2.11	3	2
1:A:1:GLY:HA3	1:A:34:GLY:HA3	0.44	1.89	2	3
1:A:3:CYS:HA	1:A:36:TYR:CE1	0.44	2.48	17	2
1:A:31:ASP:CG	1:A:37:ARG:HB2	0.44	2.33	8	1
1:A:3:CYS:HB2	1:A:36:TYR:N	0.44	2.27	17	1
1:A:31:ASP:CG	1:A:37:ARG:HD2	0.44	2.32	17	1
1:A:2:PRO:HA	1:A:5:ARG:CD	0.44	2.42	16	1
1:A:31:ASP:CG	1:A:33:ARG:HG3	0.44	2.32	8	1
1:A:2:PRO:HA	1:A:5:ARG:HD3	0.44	1.90	16	1
1:A:25:LEU:HG	1:A:43:SER:HB2	0.44	1.90	7	1
1:A:31:ASP:CG	1:A:32:HIS:N	0.44	2.72	19	2
1:A:40:GLN:C	1:A:41:CYS:SG	0.44	2.96	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:LEU:HG	1:A:28:PRO:O	0.44	2.13	8	2
1:A:40:GLN:HB2	1:A:53:TRP:NE1	0.43	2.28	20	4
1:A:25:LEU:HG	1:A:25:LEU:O	0.43	2.11	7	1
1:A:5:ARG:HG3	1:A:6:HIS:N	0.43	2.28	7	1
1:A:26:TYR:CD1	1:A:41:CYS:O	0.43	2.71	9	2
1:A:2:PRO:HD2	1:A:35:PHE:CD1	0.43	2.49	16	1
1:A:13:GLN:O	1:A:17:GLU:HG2	0.43	2.13	4	1
1:A:35:PHE:HB3	1:A:57:ARG:O	0.43	2.13	8	1
1:A:56:ASP:N	1:A:62:LEU:HG	0.43	2.28	11	1
1:A:32:HIS:CE1	1:A:33:ARG:CD	0.43	3.01	14	1
1:A:10:VAL:HG11	1:A:27:VAL:HG12	0.43	1.90	15	1
1:A:2:PRO:HD2	1:A:35:PHE:CE1	0.43	2.49	4	1
1:A:4:ARG:HD2	1:A:4:ARG:C	0.43	2.34	3	1
1:A:33:ARG:O	1:A:33:ARG:HG3	0.43	2.13	12	2
1:A:31:ASP:HB2	1:A:37:ARG:CG	0.43	2.44	19	1
1:A:3:CYS:HA	1:A:36:TYR:CZ	0.42	2.49	6	2
1:A:33:ARG:O	1:A:33:ARG:CG	0.42	2.66	12	2
1:A:3:CYS:HB2	1:A:36:TYR:CG	0.42	2.49	4	2
1:A:31:ASP:HB3	1:A:37:ARG:CD	0.42	2.43	8	1
1:A:40:GLN:C	1:A:52:CYS:SG	0.42	2.98	6	1
1:A:10:VAL:HG11	1:A:27:VAL:CG1	0.42	2.44	15	1
1:A:39:ARG:HD2	1:A:39:ARG:C	0.42	2.35	1	1
1:A:58:MET:O	1:A:58:MET:HG3	0.42	2.13	16	1
1:A:17:GLU:C	1:A:25:LEU:HD11	0.42	2.35	17	1
1:A:27:VAL:O	1:A:41:CYS:HB2	0.42	2.15	6	1
1:A:3:CYS:CB	1:A:34:GLY:O	0.42	2.68	5	2
1:A:36:TYR:HB2	1:A:59:GLY:CA	0.42	2.44	6	2
1:A:17:GLU:HB3	1:A:25:LEU:HD13	0.42	1.91	12	1
1:A:40:GLN:CB	1:A:53:TRP:CE2	0.42	3.03	8	1
1:A:33:ARG:CD	1:A:33:ARG:N	0.41	2.80	11	1
1:A:31:ASP:HB3	1:A:37:ARG:HD3	0.41	1.90	4	1
1:A:11:LEU:CA	1:A:14:LEU:HD23	0.41	2.31	8	3
1:A:26:TYR:CD1	1:A:27:VAL:N	0.41	2.89	8	1
1:A:26:TYR:CD1	1:A:26:TYR:C	0.41	2.93	11	1
1:A:11:LEU:O	1:A:15:GLN:HB2	0.41	2.15	11	1
1:A:9:SER:O	1:A:13:GLN:HB2	0.41	2.15	14	1
1:A:26:TYR:CE1	1:A:40:GLN:HA	0.41	2.51	8	1
1:A:14:LEU:HA	1:A:25:LEU:HD13	0.41	1.92	17	1
1:A:26:TYR:HB2	1:A:42:ARG:HA	0.41	1.93	8	2
1:A:39:ARG:CD	1:A:52:CYS:CB	0.41	2.99	6	1
1:A:40:GLN:CD	1:A:55:VAL:HG11	0.41	2.36	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:VAL:O	1:A:14:LEU:HB3	0.41	2.16	9	1
1:A:56:ASP:OD2	1:A:60:LYS:HB3	0.41	2.16	9	1
1:A:53:TRP:CD1	1:A:55:VAL:CG1	0.40	3.04	11	1
1:A:16:THR:HG22	1:A:17:GLU:CG	0.40	2.46	11	1
1:A:1:GLY:O	1:A:5:ARG:HD3	0.40	2.16	14	1
1:A:40:GLN:HB2	1:A:55:VAL:CG1	0.40	2.45	16	1
1:A:14:LEU:C	1:A:14:LEU:CD1	0.40	2.89	18	1
1:A:40:GLN:CG	1:A:55:VAL:CG1	0.40	2.94	11	1
1:A:31:ASP:CG	1:A:33:ARG:HD3	0.40	2.36	14	1
1:A:6:HIS:CG	1:A:28:PRO:HG3	0.40	2.51	8	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	48/107 (45%)	43±1 (90±3%)	4±2 (9±3%)	0±0 (1±1%)	29	74
All	All	960/2140 (45%)	864 (90%)	90 (9%)	6 (1%)	29	74

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	24	THR	6

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	45/92 (49%)	30±3 (68±7%)	15±3 (32±7%)	1	13
All	All	900/1840 (49%)	609 (68%)	291 (32%)	1	13

All 38 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	57	ARG	14
1	A	29	ASN	13
1	A	11	LEU	12
1	A	42	ARG	12
1	A	4	ARG	12
1	A	14	LEU	12
1	A	33	ARG	11
1	A	54	CYS	11
1	A	58	MET	11
1	A	38	LYS	11
1	A	24	THR	10
1	A	37	ARG	10
1	A	7	LEU	9
1	A	8	ASP	9
1	A	26	TYR	9
1	A	31	ASP	9
1	A	52	CYS	9
1	A	60	LYS	9
1	A	30	CYS	9
1	A	32	HIS	9
1	A	56	ASP	9
1	A	13	GLN	8
1	A	39	ARG	8
1	A	5	ARG	8
1	A	25	LEU	6
1	A	43	SER	6
1	A	15	GLN	5
1	A	61	SER	5
1	A	40	GLN	5
1	A	16	THR	4
1	A	12	GLN	3
1	A	6	HIS	3
1	A	36	TYR	2
1	A	3	CYS	2
1	A	35	PHE	2
1	A	62	LEU	2
1	A	17	GLU	1
1	A	55	VAL	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