



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 07:53 PM BST

PDB ID : 2EDQ
Title : Solution structure of the ig-like domain (3713-3806) of human obscurin
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Deposited on : 2007-02-14

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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

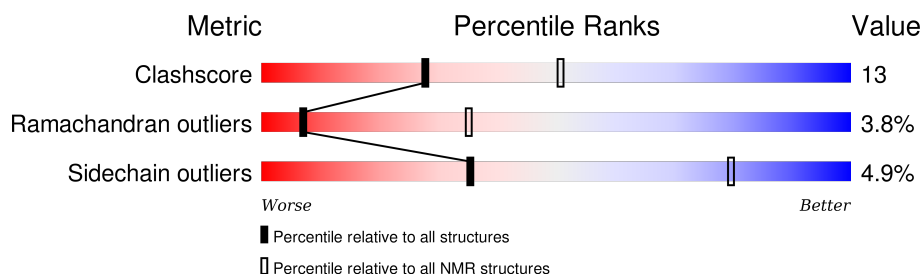
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	107	<div> <div>64%</div> <div>15%</div> <div>21%</div> </div>

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:9-A:49, A:53-A:95 (84)	0.26	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1571 atoms, of which 771 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Obscurin.

Mol	Chain	Residues	Atoms						Trace
1	A	107	Total	C	H	N	O	S	0
			1571	482	771	150	164	4	

There are 13 discrepancies between the modelled and reference sequences:

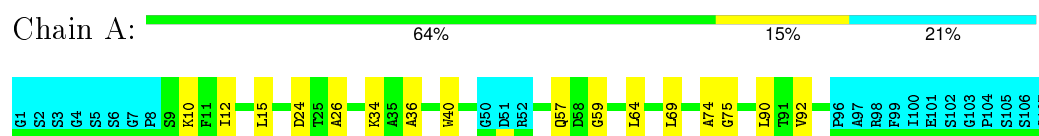
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP Q5VST9
A	2	SER	-	CLONING ARTIFACT	UNP Q5VST9
A	3	SER	-	CLONING ARTIFACT	UNP Q5VST9
A	4	GLY	-	CLONING ARTIFACT	UNP Q5VST9
A	5	SER	-	CLONING ARTIFACT	UNP Q5VST9
A	6	SER	-	CLONING ARTIFACT	UNP Q5VST9
A	7	GLY	-	CLONING ARTIFACT	UNP Q5VST9
A	102	SER	-	CLONING ARTIFACT	UNP Q5VST9
A	103	GLY	-	CLONING ARTIFACT	UNP Q5VST9
A	104	PRO	-	CLONING ARTIFACT	UNP Q5VST9
A	105	SER	-	CLONING ARTIFACT	UNP Q5VST9
A	106	SER	-	CLONING ARTIFACT	UNP Q5VST9
A	107	GLY	-	CLONING ARTIFACT	UNP Q5VST9

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Obscurin

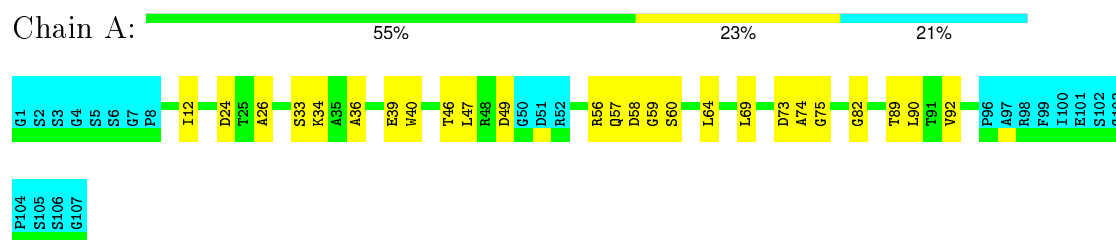


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

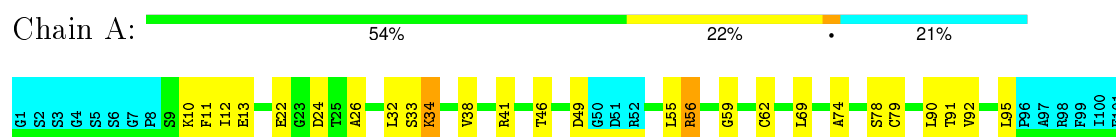
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Obscurin



4.2.2 Score per residue for model 2

- Molecule 1: Obscurin



S102
G103
P104
S105
S106
G107

4.2.3 Score per residue for model 3

- Molecule 1: Obscurin

Chain A: 

G1 S2 S3 S4 S5 S6 S7 S8 L28 V38 V39 V40 G43 H44 E45 T46 L47 D49 G50 D51 R52 L55 G59 C62 E63 L64 A74 G75 T89 L90 T91 V92 P96 A97 R98 F99 I100 E101 S102 G103 P104 S105 S106 G107

4.2.4 Score per residue for model 4

- Molecule 1: Obscurin

Chain A: 

G1 S2 S3 G4 S5 S6 S7 S8 S9 F10 F11 F12 L15 E22 L28 E31 K34 A35 A36 R37 V38 E39 W40 L47 G50 D51 R52 R53 Q57 D58 G59 C62 E63 L64 A70 D73 A74 C79 V80 C81 T86 L90 T91 V92 L95

P96 A97 R98 F99 I100 E101 S102 G103 P104 S105 S106 G107

4.2.5 Score per residue for model 5

- Molecule 1: Obscurin

Chain A: 

G1 S2 S3 S4 S5 S6 S7 S8 F11 I12 E13 G14 M17 E18 E19 D24 T25 A26 T27 L28 S33 K34 V38 E39 W40 G50 D51 R52 R53 S54 Q57 D58 G59 S60 R61 C62 E63 L64 I66 L69 A74 C79 L90 T91 V92 P96 A97

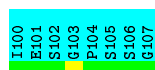
R98 F99 I100 E101 S102 G103 P104 S105 S106 G107

4.2.6 Score per residue for model 6

- Molecule 1: Obscurin

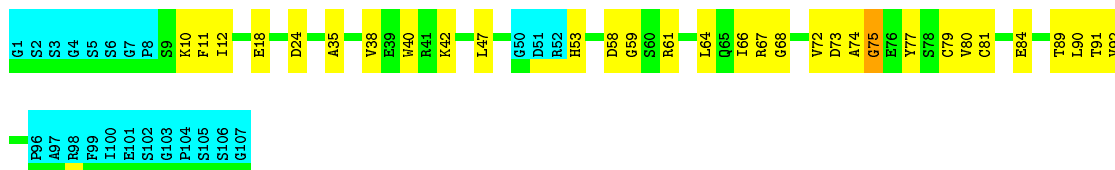
Chain A: 

G1 S2 S3 S4 S5 S6 S7 S8 E13 G14 L15 L16 W17 E18 G22 G23 A26 T27 L28 L32 S33 K34 A35 A36 F37 V38 E39 W40 G50 D51 R52 R53 H53 Q57 C62 E63 L64 L69 A74 G75 G82 T89 L90 T91 V92 P96 A97 R98 F99



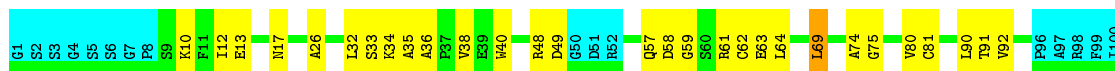
4.2.7 Score per residue for model 7

- Molecule 1: Obscurin



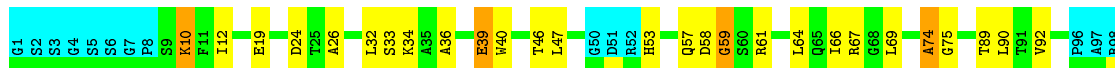
4.2.8 Score per residue for model 8

- Molecule 1: Obscurin



4.2.9 Score per residue for model 9

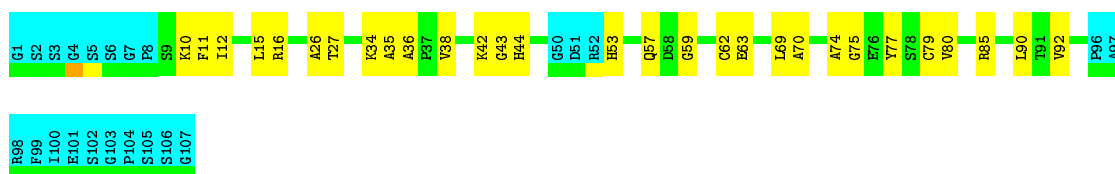
- Molecule 1: Obscurin



4.2.10 Score per residue for model 10

- Molecule 1: Obscurin

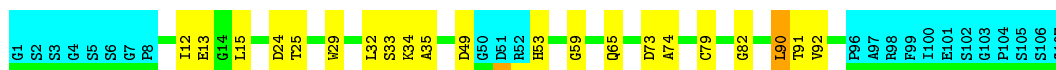




4.2.11 Score per residue for model 11

- Molecule 1: Obscurin

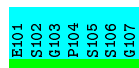
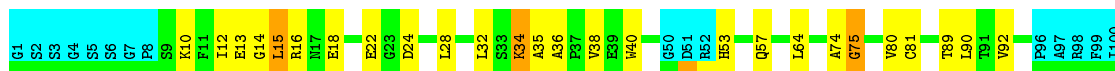
Chain A: 59% 19% 21%



4.2.12 Score per residue for model 12

- Molecule 1: Obscurin

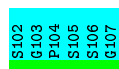
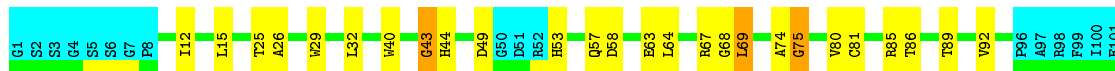
Chain A: 54% 21% 21%



4.2.13 Score per residue for model 13

- Molecule 1: Obscurin

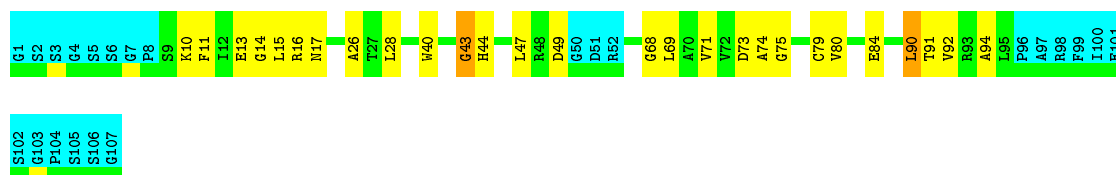
Chain A: 54% 21% 21%



4.2.14 Score per residue for model 14

- Molecule 1: Obscurin

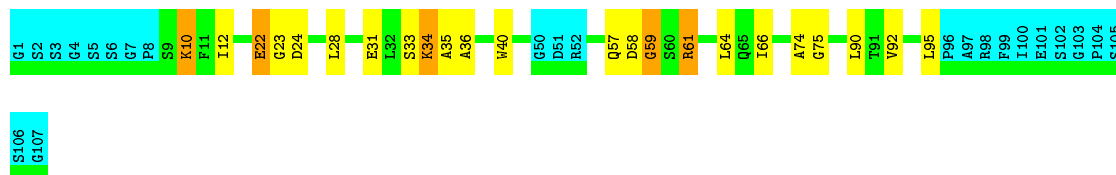
Chain A: 53% 23% 21%



4.2.15 Score per residue for model 15

- Molecule 1: Obscurin

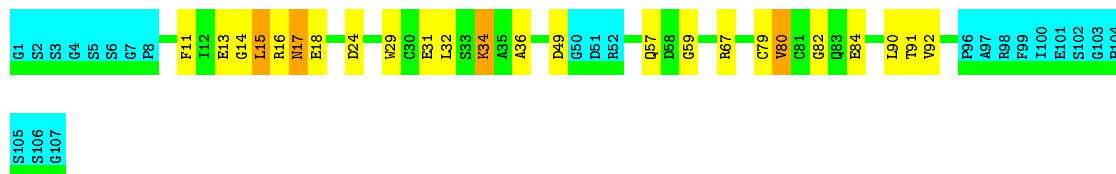
Chain A: 57% 17% 5% 21%



4.2.16 Score per residue for model 16

- Molecule 1: Obscurin

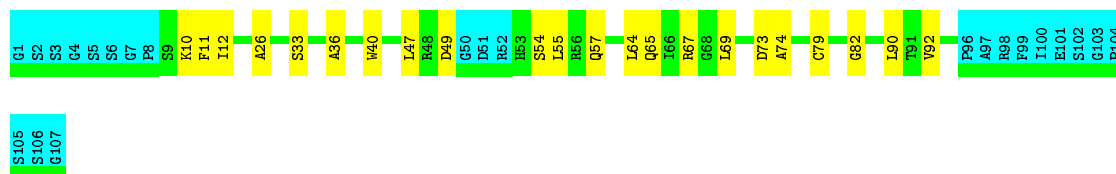
Chain A: 56% 19% 1% 21%



4.2.17 Score per residue for model 17

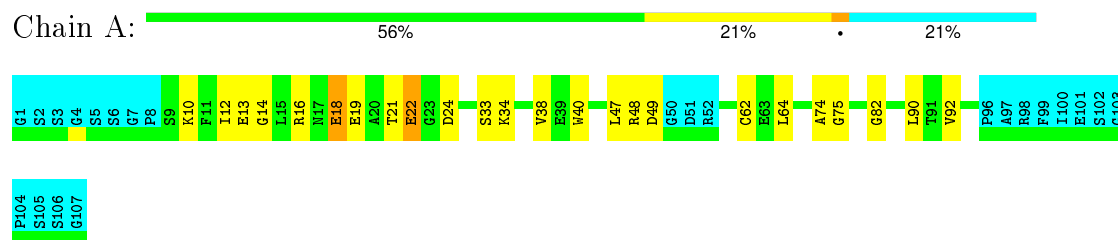
- Molecule 1: Obscurin

Chain A: 58% 21% 21%



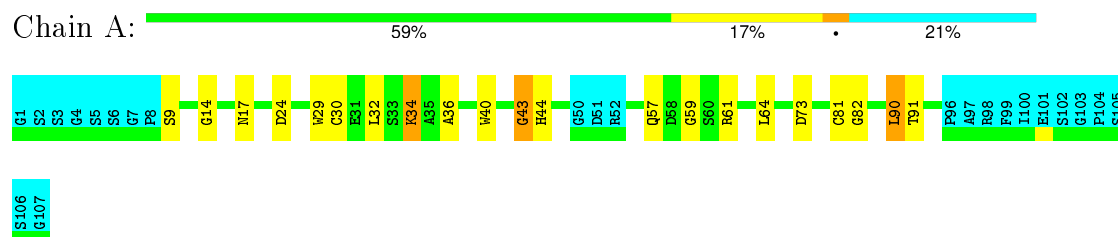
4.2.18 Score per residue for model 18

- Molecule 1: Obscurin



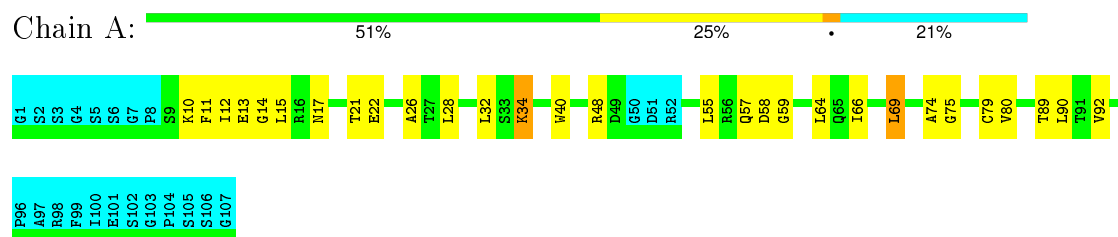
4.2.19 Score per residue for model 19

- Molecule 1: Obscurin



4.2.20 Score per residue for model 20

- Molecule 1: Obscurin



5 Refinement protocol and experimental data overview

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

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

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. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

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	650	636	634	16±3
All	All	13000	12720	12680	326

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:ALA:HB2	1:A:92:VAL:HG23	0.93	1.36	12	18
1:A:74:ALA:HB2	1:A:92:VAL:CG2	0.82	2.04	11	12
1:A:90:LEU:HD13	1:A:91:THR:N	0.81	1.90	8	7
1:A:40:TRP:CE3	1:A:64:LEU:HD22	0.79	2.13	13	15
1:A:39:GLU:OE1	1:A:46:THR:HG23	0.76	1.81	9	1
1:A:80:VAL:HG23	1:A:84:GLU:O	0.75	1.81	16	3
1:A:32:LEU:HD23	1:A:34:LYS:O	0.74	1.81	12	9
1:A:26:ALA:HB2	1:A:69:LEU:HD21	0.72	1.60	5	6
1:A:10:LYS:O	1:A:12:ILE:HD13	0.71	1.84	9	7
1:A:38:VAL:HG11	1:A:62:CYS:SG	0.71	2.25	8	6
1:A:40:TRP:HB3	1:A:47:LEU:HD12	0.70	1.63	18	7
1:A:28:LEU:HD11	1:A:90:LEU:CD1	0.70	2.16	15	5
1:A:32:LEU:HD21	1:A:81:CYS:SG	0.66	2.31	13	2
1:A:74:ALA:HB1	1:A:90:LEU:O	0.64	1.91	1	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:ALA:HB2	1:A:69:LEU:HD11	0.64	1.70	10	5
1:A:40:TRP:CE3	1:A:64:LEU:CD2	0.63	2.81	13	8
1:A:39:GLU:CD	1:A:46:THR:HG23	0.63	2.14	9	1
1:A:22:GLU:O	1:A:95:LEU:HD11	0.62	1.95	15	2
1:A:26:ALA:CB	1:A:69:LEU:HD21	0.62	2.24	8	3
1:A:15:LEU:HD22	1:A:28:LEU:HD12	0.61	1.73	4	1
1:A:74:ALA:CB	1:A:92:VAL:HG23	0.60	2.25	11	1
1:A:11:PHE:CZ	1:A:79:CYS:O	0.60	2.55	16	9
1:A:80:VAL:HG22	1:A:85:ARG:HG3	0.60	1.73	13	1
1:A:11:PHE:CE2	1:A:79:CYS:O	0.58	2.56	10	3
1:A:22:GLU:OE1	1:A:95:LEU:HD12	0.58	1.98	2	1
1:A:75:GLY:O	1:A:89:THR:HG23	0.57	2.00	13	8
1:A:12:ILE:HD11	1:A:33:SER:CB	0.57	2.30	15	4
1:A:15:LEU:HD11	1:A:79:CYS:HB2	0.57	1.75	10	2
1:A:15:LEU:HD12	1:A:86:THR:HG23	0.57	1.77	13	2
1:A:29:TRP:CE2	1:A:61:ARG:NH2	0.56	2.73	19	1
1:A:90:LEU:CD1	1:A:92:VAL:CG2	0.56	2.83	18	1
1:A:90:LEU:CD1	1:A:92:VAL:HG23	0.56	2.30	16	1
1:A:70:ALA:HB3	1:A:73:ASP:OD1	0.55	2.02	4	1
1:A:29:TRP:CD2	1:A:61:ARG:NH2	0.54	2.75	19	1
1:A:19:GLU:OE1	1:A:91:THR:HG21	0.54	2.03	5	1
1:A:12:ILE:HD11	1:A:33:SER:N	0.53	2.19	8	2
1:A:53:HIS:NE2	1:A:66:ILE:HG23	0.53	2.18	9	2
1:A:18:GLU:HB2	1:A:28:LEU:HD21	0.53	1.81	6	1
1:A:12:ILE:HD11	1:A:33:SER:HB2	0.52	1.81	2	3
1:A:39:GLU:OE2	1:A:46:THR:HG21	0.52	2.05	1	1
1:A:66:ILE:HG22	1:A:66:ILE:O	0.52	2.05	15	2
1:A:28:LEU:HD11	1:A:90:LEU:HD11	0.51	1.81	20	5
1:A:18:GLU:HB3	1:A:90:LEU:HD12	0.51	1.81	12	2
1:A:57:GLN:NE2	1:A:59:GLY:O	0.51	2.44	10	1
1:A:9:SER:O	1:A:32:LEU:HD11	0.51	2.05	19	1
1:A:36:ALA:O	1:A:57:GLN:NE2	0.50	2.44	15	10
1:A:38:VAL:HG21	1:A:62:CYS:SG	0.50	2.46	18	3
1:A:32:LEU:CD2	1:A:34:LYS:O	0.50	2.60	2	4
1:A:34:LYS:O	1:A:36:ALA:N	0.50	2.45	15	2
1:A:12:ILE:HD13	1:A:12:ILE:N	0.49	2.22	11	3
1:A:74:ALA:CB	1:A:90:LEU:O	0.49	2.61	1	3
1:A:38:VAL:CG2	1:A:62:CYS:SG	0.49	3.01	10	1
1:A:71:VAL:CG2	1:A:94:ALA:HB2	0.49	2.38	14	1
1:A:64:LEU:HD12	1:A:65:GLN:H	0.48	1.68	17	1
1:A:18:GLU:C	1:A:18:GLU:CD	0.48	2.71	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:LEU:HD12	1:A:92:VAL:HG23	0.48	1.84	16	3
1:A:39:GLU:CD	1:A:40:TRP:N	0.48	2.67	9	1
1:A:58:ASP:O	1:A:61:ARG:N	0.48	2.46	8	4
1:A:58:ASP:O	1:A:61:ARG:CB	0.48	2.62	8	3
1:A:18:GLU:O	1:A:90:LEU:HD22	0.48	2.09	7	1
1:A:18:GLU:CD	1:A:18:GLU:C	0.48	2.73	18	1
1:A:41:ARG:HG2	1:A:46:THR:HG23	0.48	1.86	2	1
1:A:49:ASP:N	1:A:55:LEU:HD13	0.47	2.24	3	2
1:A:43:GLY:O	1:A:45:GLU:N	0.47	2.47	3	1
1:A:22:GLU:OE2	1:A:23:GLY:N	0.47	2.47	15	2
1:A:40:TRP:CB	1:A:47:LEU:HD12	0.47	2.38	18	2
1:A:25:THR:HG23	1:A:67:ARG:HA	0.47	1.85	13	1
1:A:74:ALA:HB2	1:A:92:VAL:CB	0.47	2.39	11	2
1:A:38:VAL:HG21	1:A:62:CYS:CB	0.47	2.40	18	1
1:A:38:VAL:HG12	1:A:81:CYS:HB2	0.47	1.85	12	2
1:A:39:GLU:OE2	1:A:46:THR:CG2	0.47	2.62	1	1
1:A:9:SER:O	1:A:32:LEU:CD1	0.47	2.63	19	1
1:A:54:SER:O	1:A:64:LEU:HD12	0.47	2.10	5	1
1:A:13:GLU:HG2	1:A:29:TRP:CH2	0.46	2.46	11	2
1:A:18:GLU:CD	1:A:19:GLU:N	0.46	2.68	18	1
1:A:55:LEU:HD12	1:A:55:LEU:N	0.46	2.25	17	1
1:A:48:ARG:C	1:A:55:LEU:HD13	0.46	2.31	20	1
1:A:40:TRP:CZ3	1:A:64:LEU:HB3	0.46	2.46	17	1
1:A:12:ILE:N	1:A:12:ILE:HD13	0.46	2.25	20	2
1:A:58:ASP:O	1:A:59:GLY:C	0.45	2.54	15	7
1:A:74:ALA:CA	1:A:90:LEU:O	0.45	2.64	4	1
1:A:63:GLU:C	1:A:63:GLU:OE1	0.45	2.55	3	1
1:A:14:GLY:O	1:A:15:LEU:C	0.45	2.55	14	5
1:A:38:VAL:HG12	1:A:81:CYS:HB3	0.45	1.88	8	2
1:A:13:GLU:O	1:A:14:GLY:C	0.45	2.55	20	5
1:A:70:ALA:O	1:A:92:VAL:HG11	0.45	2.11	10	1
1:A:16:ARG:O	1:A:17:ASN:C	0.45	2.55	16	2
1:A:38:VAL:CG1	1:A:62:CYS:SG	0.45	3.03	8	2
1:A:43:GLY:O	1:A:44:HIS:C	0.45	2.55	13	5
1:A:58:ASP:N	1:A:61:ARG:O	0.44	2.49	9	1
1:A:29:TRP:CD2	1:A:29:TRP:O	0.44	2.70	13	1
1:A:34:LYS:O	1:A:35:ALA:C	0.44	2.56	11	2
1:A:40:TRP:CD2	1:A:64:LEU:HB2	0.44	2.48	9	3
1:A:19:GLU:CD	1:A:19:GLU:C	0.44	2.76	9	1
1:A:12:ILE:HD11	1:A:33:SER:HB3	0.44	1.90	11	2
1:A:61:ARG:NH2	1:A:63:GLU:OE1	0.44	2.51	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:ARG:NH1	1:A:17:ASN:O	0.44	2.51	6	1
1:A:12:ILE:HD11	1:A:33:SER:CA	0.43	2.43	8	4
1:A:21:THR:O	1:A:22:GLU:C	0.43	2.56	18	2
1:A:69:LEU:HD23	1:A:73:ASP:OD2	0.43	2.12	17	1
1:A:49:ASP:O	1:A:49:ASP:CG	0.43	2.57	13	1
1:A:90:LEU:CD1	1:A:92:VAL:HG22	0.43	2.44	18	1
1:A:15:LEU:HD21	1:A:40:TRP:CH2	0.42	2.48	20	1
1:A:42:LYS:HD2	1:A:77:TYR:CE2	0.42	2.49	10	1
1:A:85:ARG:CZ	1:A:85:ARG:HB3	0.42	2.45	10	1
1:A:43:GLY:C	1:A:44:HIS:CD2	0.42	2.93	13	1
1:A:48:ARG:O	1:A:49:ASP:C	0.42	2.58	18	1
1:A:66:ILE:O	1:A:66:ILE:HG22	0.42	2.15	9	1
1:A:40:TRP:CE2	1:A:64:LEU:HB2	0.41	2.50	8	1
1:A:42:LYS:HB2	1:A:47:LEU:HD21	0.41	1.92	7	1
1:A:27:THR:HG21	1:A:63:GLU:OE2	0.41	2.16	10	1
1:A:29:TRP:CE3	1:A:30:CYS:N	0.41	2.88	19	1
1:A:90:LEU:HD12	1:A:92:VAL:CG2	0.41	2.44	18	1
1:A:12:ILE:CD1	1:A:33:SER:HB2	0.41	2.45	15	1
1:A:66:ILE:HD13	1:A:77:TYR:OH	0.41	2.16	7	1
1:A:55:LEU:N	1:A:55:LEU:CD1	0.41	2.83	17	1
1:A:80:VAL:CG2	1:A:84:GLU:O	0.41	2.61	16	1
1:A:56:ARG:CZ	1:A:56:ARG:HB3	0.41	2.45	1	1
1:A:58:ASP:O	1:A:60:SER:N	0.41	2.53	1	1
1:A:38:VAL:HG21	1:A:62:CYS:HB3	0.41	1.93	18	1
1:A:15:LEU:HD22	1:A:28:LEU:HD22	0.40	1.92	14	1
1:A:25:THR:CG2	1:A:65:GLN:HG2	0.40	2.46	11	1
1:A:48:ARG:CZ	1:A:48:ARG:HB3	0.40	2.46	8	1
1:A:36:ALA:O	1:A:57:GLN:OE1	0.40	2.40	8	1
1:A:56:ARG:CZ	1:A:56:ARG:HB2	0.40	2.46	2	1
1:A:72:VAL:HG23	1:A:73:ASP:N	0.40	2.31	7	1
1:A:19:GLU:O	1:A:19:GLU:CD	0.40	2.60	9	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	84/107 (79%)	69±2 (82±3%)	12±3 (14±3%)	3±1 (4±2%)	7	35
All	All	1680/2140 (79%)	1380 (82%)	237 (14%)	63 (4%)	7	35

All 15 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	24	ASP	10
1	A	75	GLY	9
1	A	59	GLY	8
1	A	82	GLY	7
1	A	35	ALA	5
1	A	43	GLY	4
1	A	17	ASN	3
1	A	14	GLY	3
1	A	15	LEU	3
1	A	69	LEU	3
1	A	22	GLU	2
1	A	74	ALA	2
1	A	68	GLY	2
1	A	47	LEU	1
1	A	44	HIS	1

6.3.2 Protein sidechains ⓘ

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	69/85 (81%)	66±1 (95±2%)	3±1 (5±2%)	35	79
All	All	1380/1700 (81%)	1312 (95%)	68 (5%)	35	79

All 22 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	34	LYS	9
1	A	10	LYS	8
1	A	49	ASP	6

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Mol	Chain	Res	Type	Models (Total)
1	A	80	VAL	6
1	A	73	ASP	5
1	A	16	ARG	4
1	A	13	GLU	4
1	A	31	GLU	3
1	A	57	GLN	3
1	A	67	ARG	3
1	A	90	LEU	3
1	A	17	ASN	2
1	A	63	GLU	2
1	A	18	GLU	2
1	A	22	GLU	1
1	A	58	ASP	1
1	A	56	ARG	1
1	A	54	SER	1
1	A	39	GLU	1
1	A	61	ARG	1
1	A	24	ASP	1
1	A	78	SER	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided