



Full wwPDB NMR Structure Validation Report ⓘ

Mar 4, 2026 – 09:12 PM UTC

PDB ID : 2EKI / pdb_00002eki
Title : Solution structures of the TGS domain of human developmentally-regulated GTP-binding protein 1
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Deposited on : 2007-03-23

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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

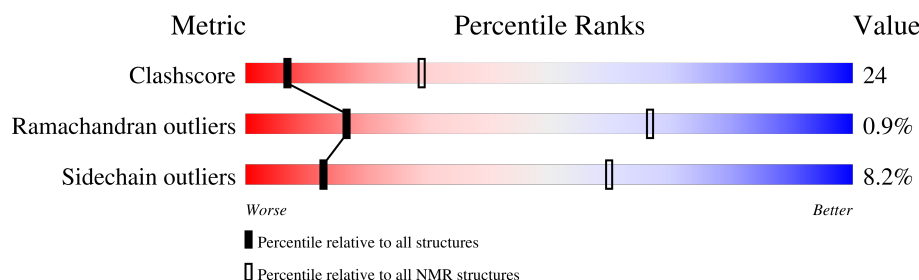
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	93	

2 Ensemble composition and analysis

This entry contains 20 models. Model 12 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:10-A:87 (78)	0.46	12

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1483 atoms, of which 753 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Developmentally-regulated GTP-binding protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	93	Total	C	H	N	O	S	0
			1483	469	753	123	136	2	

There are 13 discrepancies between the modelled and reference sequences:

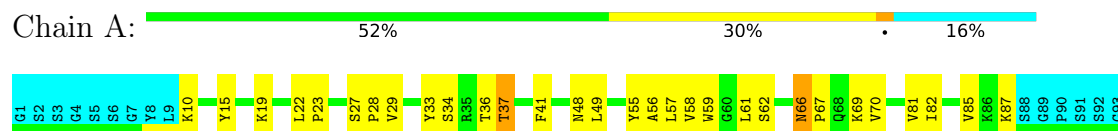
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9Y295
A	2	SER	-	expression tag	UNP Q9Y295
A	3	SER	-	expression tag	UNP Q9Y295
A	4	GLY	-	expression tag	UNP Q9Y295
A	5	SER	-	expression tag	UNP Q9Y295
A	6	SER	-	expression tag	UNP Q9Y295
A	7	GLY	-	expression tag	UNP Q9Y295
A	88	SER	-	expression tag	UNP Q9Y295
A	89	GLY	-	expression tag	UNP Q9Y295
A	90	PRO	-	expression tag	UNP Q9Y295
A	91	SER	-	expression tag	UNP Q9Y295
A	92	SER	-	expression tag	UNP Q9Y295
A	93	GLY	-	expression tag	UNP Q9Y295

4 Residue-property plots

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: Developmentally-regulated GTP-binding protein 1

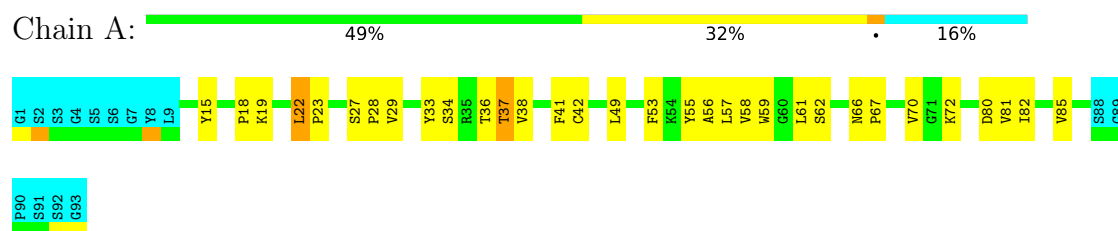


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

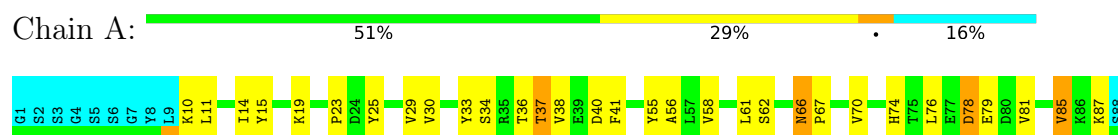
4.2.1 Score per residue for model 1

- Molecule 1: Developmentally-regulated GTP-binding protein 1



4.2.2 Score per residue for model 2

- Molecule 1: Developmentally-regulated GTP-binding protein 1



G89
P90
S91
S92
G93

4.2.3 Score per residue for model 3

- Molecule 1: Developmentally-regulated GTP-binding protein 1

Chain A: 51% 29% 1% 16%

G1 S2 S3 S4 S5 S6 S7 S8 S9 K10 Y15 G20 P23 D24 Y25 T26 S27 P28 Y33 S34 R35 T36 T37 F41 M48 L49 Y55 A56 L57 V58 L61 N66 P67 Q68 K69 V70 D78 E79 D80 V81 I82 Q83 I84 V85 S88 G89 P90 S91

S92
G93

4.2.4 Score per residue for model 4

- Molecule 1: Developmentally-regulated GTP-binding protein 1

Chain A: 46% 37% 1% 16%

G1 S2 S3 S4 S5 S6 S7 S8 S9 K10 L11 L14 Y15 P18 K19 L22 P28 V29 Y30 V33 S34 R35 T36 T37 V38 E39 D40 F41 C42 M43 M48 Y55 A56 L57 V58 W59 G60 L61 K64 H65 N66 P67 V70 D80 V81 I82 V85

S88
G89
P90
S91
S92
G93

4.2.5 Score per residue for model 5

- Molecule 1: Developmentally-regulated GTP-binding protein 1

Chain A: 47% 33% 1% 16%

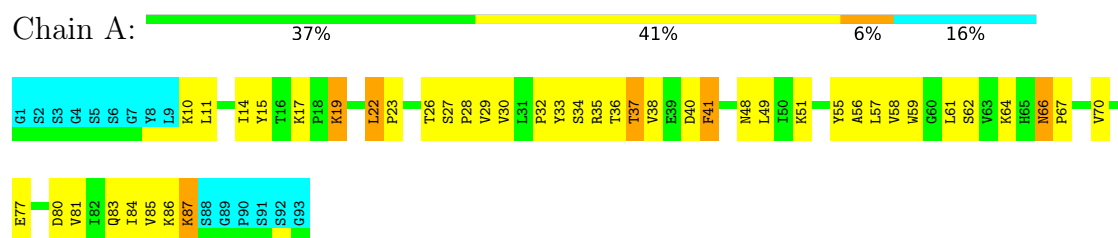
G1 S2 S3 S4 S5 S6 S7 S8 S9 K10 L11 V12 R13 L14 Y15 T16 K17 L22 P23 D24 Y25 T26 S27 P28 L31 P32 Y33 S34 R35 T36 T37 F41 K44 L49 Y55 A56 L57 V58 W59 G60 S62 N66 P67 V70 G71 K72 D78 V81 I82

Q83
I84 V85 K86 K87 S88 G89 P90 S91 S92 G93

4.2.6 Score per residue for model 6

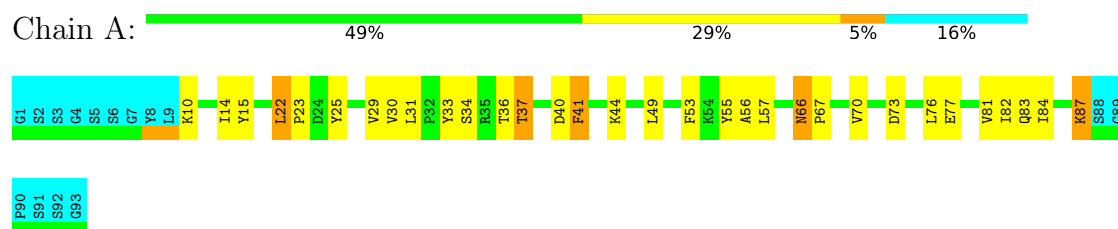
- Molecule 1: Developmentally-regulated GTP-binding protein 1

Chain A: 47% 31% 5% 16%



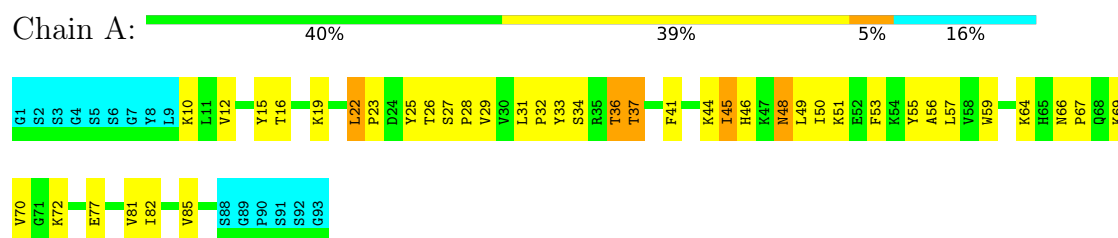
4.2.11 Score per residue for model 11

- Molecule 1: Developmentally-regulated GTP-binding protein 1



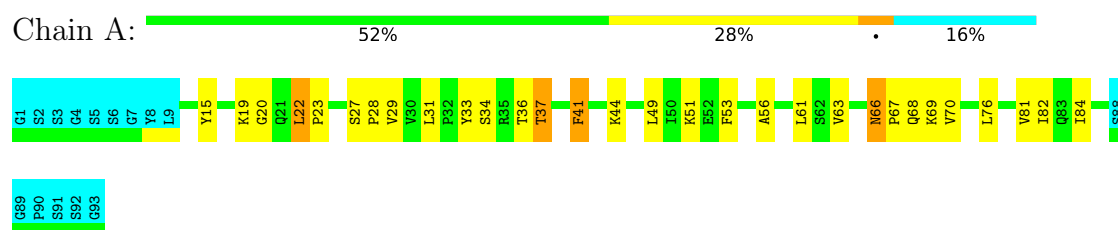
4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Developmentally-regulated GTP-binding protein 1



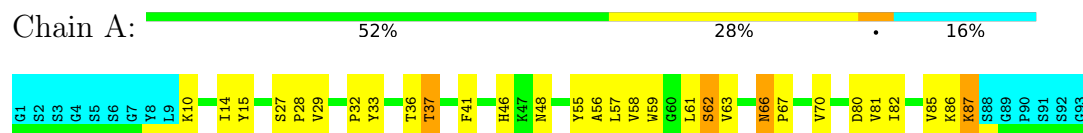
4.2.13 Score per residue for model 13

- Molecule 1: Developmentally-regulated GTP-binding protein 1



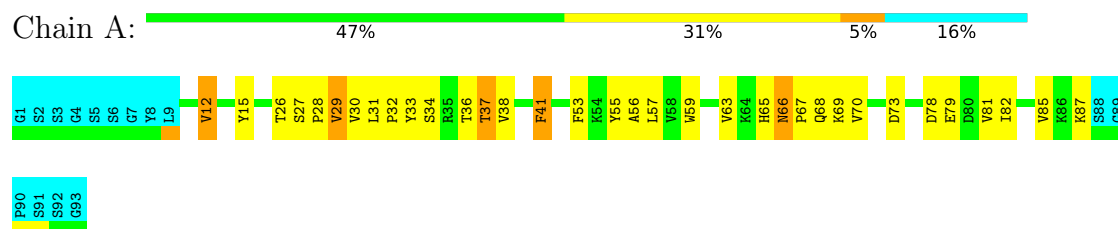
4.2.18 Score per residue for model 18

- Molecule 1: Developmentally-regulated GTP-binding protein 1



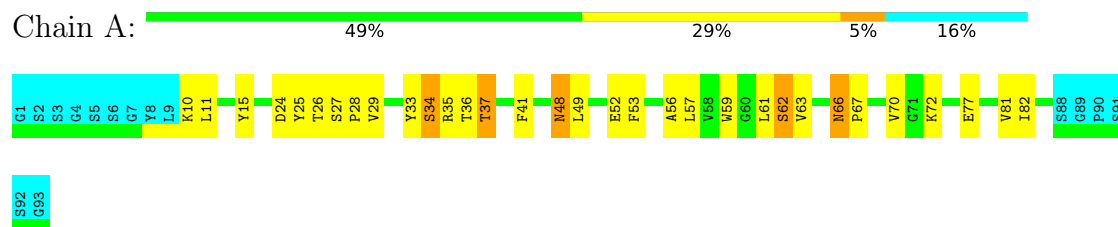
4.2.19 Score per residue for model 19

- Molecule 1: Developmentally-regulated GTP-binding protein 1



4.2.20 Score per residue for model 20

- Molecule 1: Developmentally-regulated GTP-binding protein 1



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, 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.

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	641	676	673	32±6
All	All	12820	13520	13460	639

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 24.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:ALA:HB3	1:A:70:VAL:CG2	0.87	2.00	7	11
1:A:56:ALA:O	1:A:70:VAL:HG22	0.82	1.74	16	17
1:A:55:TYR:CE1	1:A:85:VAL:HG21	0.81	2.10	1	2
1:A:55:TYR:CZ	1:A:85:VAL:HG11	0.75	2.17	2	4
1:A:15:TYR:HB2	1:A:81:VAL:HG22	0.74	1.57	7	19
1:A:10:LYS:C	1:A:11:LEU:HD22	0.74	2.08	2	4
1:A:55:TYR:CE1	1:A:85:VAL:HG11	0.74	2.17	2	6
1:A:36:THR:O	1:A:37:THR:HG23	0.71	1.85	10	20
1:A:55:TYR:CZ	1:A:85:VAL:HG21	0.69	2.23	19	10
1:A:55:TYR:CE2	1:A:85:VAL:HG21	0.69	2.23	18	7
1:A:14:ILE:O	1:A:29:VAL:HG12	0.68	1.89	8	4
1:A:57:LEU:HD12	1:A:83:GLN:OE1	0.68	1.88	17	2
1:A:63:VAL:HG23	1:A:66:ASN:ND2	0.67	2.03	17	3
1:A:29:VAL:HG11	1:A:41:PHE:CE2	0.67	2.24	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:ALA:HB3	1:A:70:VAL:HG23	0.67	1.67	7	3
1:A:68:GLN:OE1	1:A:70:VAL:HG13	0.67	1.90	13	1
1:A:41:PHE:C	1:A:41:PHE:CD1	0.67	2.72	11	20
1:A:56:ALA:HB1	1:A:82:ILE:HD11	0.66	1.65	5	6
1:A:13:ARG:O	1:A:14:ILE:HD13	0.65	1.91	6	1
1:A:31:LEU:HD21	1:A:44:LYS:HG3	0.65	1.68	11	5
1:A:11:LEU:HD12	1:A:30:VAL:CG1	0.65	2.21	17	5
1:A:63:VAL:HG12	1:A:68:GLN:NE2	0.65	2.07	19	2
1:A:56:ALA:CB	1:A:82:ILE:HD11	0.64	2.21	5	8
1:A:55:TYR:CD1	1:A:85:VAL:HG21	0.62	2.29	1	1
1:A:32:PRO:O	1:A:36:THR:HG23	0.61	1.95	4	3
1:A:46:HIS:CG	1:A:48:ASN:ND2	0.61	2.68	14	1
1:A:49:LEU:HD21	1:A:84:ILE:HG21	0.60	1.72	13	7
1:A:63:VAL:CG2	1:A:66:ASN:ND2	0.60	2.65	20	4
1:A:65:HIS:C	1:A:66:ASN:ND2	0.60	2.60	14	1
1:A:49:LEU:HD13	1:A:86:LYS:NZ	0.60	2.12	17	1
1:A:57:LEU:O	1:A:59:TRP:CZ3	0.59	2.55	15	11
1:A:27:SER:N	1:A:28:PRO:CD	0.59	2.66	5	13
1:A:61:LEU:N	1:A:61:LEU:HD12	0.59	2.13	4	4
1:A:15:TYR:O	1:A:81:VAL:HG13	0.59	1.98	9	8
1:A:29:VAL:O	1:A:29:VAL:HG13	0.58	1.98	9	10
1:A:23:PRO:O	1:A:25:TYR:CE2	0.58	2.57	11	3
1:A:22:LEU:HD12	1:A:22:LEU:C	0.58	2.24	1	11
1:A:56:ALA:HB1	1:A:82:ILE:HG13	0.57	1.74	17	9
1:A:14:ILE:HD12	1:A:76:LEU:HD22	0.57	1.77	2	1
1:A:58:VAL:HG11	1:A:62:SER:OG	0.57	1.99	17	2
1:A:57:LEU:O	1:A:59:TRP:CE3	0.57	2.58	1	13
1:A:22:LEU:HD12	1:A:23:PRO:O	0.57	1.99	8	10
1:A:58:VAL:HG13	1:A:80:ASP:OD1	0.57	2.00	16	4
1:A:61:LEU:H	1:A:61:LEU:HD22	0.56	1.61	15	4
1:A:22:LEU:HD12	1:A:23:PRO:N	0.56	2.15	14	11
1:A:11:LEU:HD12	1:A:30:VAL:HG12	0.55	1.76	2	2
1:A:23:PRO:O	1:A:25:TYR:CE1	0.55	2.59	5	3
1:A:26:THR:C	1:A:28:PRO:CD	0.55	2.80	20	9
1:A:76:LEU:HD21	1:A:82:ILE:HD12	0.55	1.78	13	2
1:A:56:ALA:HB1	1:A:82:ILE:CD1	0.54	2.30	5	6
1:A:61:LEU:HD13	1:A:61:LEU:N	0.54	2.17	14	3
1:A:56:ALA:HB1	1:A:82:ILE:CG1	0.54	2.33	12	11
1:A:49:LEU:HD11	1:A:84:ILE:HG21	0.53	1.79	11	1
1:A:29:VAL:HG11	1:A:41:PHE:CD2	0.53	2.38	9	2
1:A:44:LYS:C	1:A:45:ILE:HD13	0.52	2.29	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:ASN:HA	1:A:67:PRO:C	0.52	2.30	14	20
1:A:66:ASN:ND2	1:A:66:ASN:N	0.52	2.57	14	2
1:A:45:ILE:HD13	1:A:45:ILE:N	0.52	2.17	12	1
1:A:14:ILE:HG13	1:A:76:LEU:HD22	0.52	1.80	11	1
1:A:55:TYR:CD2	1:A:69:LYS:HD2	0.52	2.40	15	1
1:A:58:VAL:HG13	1:A:80:ASP:CG	0.52	2.30	16	3
1:A:45:ILE:N	1:A:45:ILE:HD13	0.52	2.19	6	1
1:A:78:ASP:CG	1:A:79:GLU:N	0.51	2.67	2	1
1:A:63:VAL:CG1	1:A:68:GLN:NE2	0.51	2.73	19	1
1:A:23:PRO:O	1:A:25:TYR:CD2	0.51	2.64	3	2
1:A:48:ASN:O	1:A:48:ASN:CG	0.51	2.54	10	3
1:A:42:CYS:HA	1:A:49:LEU:HD23	0.51	1.82	1	3
1:A:63:VAL:CG2	1:A:66:ASN:OD1	0.50	2.59	14	2
1:A:38:VAL:HG11	1:A:53:PHE:CZ	0.50	2.41	6	4
1:A:32:PRO:O	1:A:33:TYR:C	0.50	2.54	9	5
1:A:33:TYR:O	1:A:34:SER:C	0.50	2.55	9	18
1:A:57:LEU:HB2	1:A:59:TRP:CH2	0.50	2.41	1	10
1:A:58:VAL:HG11	1:A:62:SER:HB3	0.50	1.83	6	1
1:A:17:LYS:HD3	1:A:59:TRP:CZ3	0.50	2.42	5	2
1:A:10:LYS:O	1:A:11:LEU:HD22	0.50	2.07	2	1
1:A:12:VAL:HG13	1:A:78:ASP:HA	0.50	1.83	8	1
1:A:66:ASN:N	1:A:66:ASN:OD1	0.50	2.45	18	3
1:A:18:PRO:O	1:A:19:LYS:C	0.50	2.55	8	2
1:A:37:THR:O	1:A:38:VAL:C	0.50	2.55	7	3
1:A:61:LEU:O	1:A:63:VAL:N	0.50	2.45	6	5
1:A:22:LEU:HD12	1:A:23:PRO:C	0.49	2.31	14	11
1:A:68:GLN:OE1	1:A:69:LYS:C	0.49	2.55	13	1
1:A:86:LYS:O	1:A:87:LYS:C	0.49	2.56	9	4
1:A:23:PRO:O	1:A:25:TYR:CD1	0.49	2.66	9	1
1:A:60:GLY:O	1:A:61:LEU:C	0.49	2.53	15	1
1:A:78:ASP:CG	1:A:79:GLU:OE2	0.49	2.55	15	1
1:A:37:THR:O	1:A:40:ASP:N	0.49	2.46	2	5
1:A:42:CYS:SG	1:A:43:MET:N	0.49	2.85	9	3
1:A:34:SER:O	1:A:35:ARG:CZ	0.49	2.60	20	1
1:A:61:LEU:O	1:A:62:SER:C	0.49	2.55	7	10
1:A:80:ASP:OD1	1:A:81:VAL:N	0.49	2.46	3	2
1:A:58:VAL:CG1	1:A:80:ASP:OD2	0.48	2.61	16	4
1:A:22:LEU:CD1	1:A:23:PRO:O	0.48	2.61	8	4
1:A:37:THR:O	1:A:39:GLU:N	0.48	2.47	7	1
1:A:14:ILE:CD1	1:A:77:GLU:O	0.48	2.62	15	2
1:A:48:ASN:ND2	1:A:48:ASN:C	0.48	2.70	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:TYR:CD2	1:A:69:LYS:HE2	0.47	2.44	8	2
1:A:46:HIS:O	1:A:49:LEU:CB	0.47	2.62	9	3
1:A:17:LYS:O	1:A:83:GLN:NE2	0.47	2.47	10	1
1:A:53:PHE:CE1	1:A:55:TYR:C	0.47	2.92	11	1
1:A:55:TYR:CE1	1:A:69:LYS:HE2	0.47	2.44	17	1
1:A:15:TYR:CE1	1:A:28:PRO:HB3	0.47	2.45	6	2
1:A:61:LEU:C	1:A:63:VAL:N	0.47	2.71	6	6
1:A:68:GLN:OE1	1:A:69:LYS:N	0.47	2.47	13	1
1:A:31:LEU:HD22	1:A:40:ASP:OD2	0.47	2.10	8	1
1:A:18:PRO:CG	1:A:22:LEU:O	0.47	2.62	4	1
1:A:19:LYS:O	1:A:19:LYS:CD	0.47	2.62	7	1
1:A:66:ASN:OD1	1:A:66:ASN:N	0.47	2.47	17	3
1:A:12:VAL:HG13	1:A:78:ASP:CA	0.47	2.40	8	1
1:A:55:TYR:CD2	1:A:69:LYS:HE3	0.46	2.45	7	1
1:A:10:LYS:HB3	1:A:33:TYR:CD2	0.46	2.46	18	4
1:A:10:LYS:HB3	1:A:33:TYR:CD1	0.46	2.46	4	3
1:A:41:PHE:O	1:A:44:LYS:N	0.46	2.48	14	1
1:A:58:VAL:HG13	1:A:80:ASP:OD2	0.46	2.09	16	1
1:A:26:THR:C	1:A:28:PRO:HD3	0.46	2.36	12	7
1:A:68:GLN:OE1	1:A:70:VAL:CG1	0.46	2.64	13	1
1:A:55:TYR:CE2	1:A:85:VAL:HG11	0.45	2.47	2	6
1:A:15:TYR:CD1	1:A:28:PRO:HB3	0.45	2.47	19	7
1:A:66:ASN:N	1:A:66:ASN:HD22	0.45	2.09	14	1
1:A:78:ASP:O	1:A:79:GLU:C	0.45	2.59	2	1
1:A:61:LEU:N	1:A:61:LEU:CD1	0.45	2.80	4	2
1:A:49:LEU:O	1:A:50:ILE:C	0.45	2.59	7	2
1:A:11:LEU:HD22	1:A:11:LEU:N	0.45	2.26	14	1
1:A:55:TYR:CG	1:A:69:LYS:HE2	0.45	2.47	3	3
1:A:49:LEU:O	1:A:53:PHE:N	0.45	2.50	20	2
1:A:12:VAL:HG12	1:A:78:ASP:HB2	0.45	1.88	16	1
1:A:65:HIS:C	1:A:66:ASN:OD1	0.45	2.60	19	1
1:A:55:TYR:CD1	1:A:85:VAL:HG11	0.45	2.47	2	1
1:A:49:LEU:HD13	1:A:86:LYS:HE2	0.45	1.88	7	2
1:A:33:TYR:O	1:A:35:ARG:N	0.45	2.50	8	4
1:A:33:TYR:C	1:A:35:ARG:N	0.44	2.74	20	3
1:A:50:ILE:HG23	1:A:51:LYS:N	0.44	2.27	12	1
1:A:15:TYR:CD1	1:A:25:TYR:HA	0.44	2.47	20	1
1:A:49:LEU:O	1:A:52:GLU:N	0.44	2.50	7	5
1:A:83:GLN:OE1	1:A:83:GLN:C	0.44	2.61	3	2
1:A:23:PRO:HG2	1:A:25:TYR:CE2	0.44	2.48	2	1
1:A:52:GLU:O	1:A:53:PHE:C	0.44	2.60	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:VAL:HG11	1:A:68:GLN:HB3	0.44	1.89	15	1
1:A:11:LEU:HD12	1:A:30:VAL:HG11	0.44	1.90	17	1
1:A:27:SER:N	1:A:28:PRO:HD3	0.43	2.28	5	2
1:A:49:LEU:C	1:A:51:LYS:N	0.43	2.76	17	3
1:A:41:PHE:O	1:A:42:CYS:C	0.43	2.61	14	1
1:A:48:ASN:O	1:A:49:LEU:C	0.43	2.61	12	2
1:A:23:PRO:HG2	1:A:25:TYR:CZ	0.43	2.48	12	2
1:A:50:ILE:CG2	1:A:51:LYS:N	0.43	2.82	12	1
1:A:11:LEU:N	1:A:11:LEU:CD2	0.43	2.82	14	1
1:A:17:LYS:CD	1:A:59:TRP:CZ3	0.43	3.01	7	1
1:A:25:TYR:OH	1:A:81:VAL:HG21	0.43	2.14	9	1
1:A:59:TRP:CZ2	1:A:67:PRO:HB3	0.43	2.48	9	2
1:A:18:PRO:O	1:A:20:GLY:N	0.43	2.52	16	1
1:A:29:VAL:CG2	1:A:31:LEU:HD21	0.43	2.43	7	1
1:A:62:SER:CB	1:A:77:GLU:CD	0.42	2.92	7	1
1:A:17:LYS:HD2	1:A:59:TRP:CZ3	0.42	2.49	15	1
1:A:10:LYS:HD3	1:A:33:TYR:CE2	0.42	2.49	18	1
1:A:77:GLU:N	1:A:77:GLU:OE1	0.42	2.52	20	1
1:A:38:VAL:HG23	1:A:74:HIS:O	0.42	2.14	14	2
1:A:78:ASP:OD1	1:A:79:GLU:N	0.42	2.52	19	1
1:A:39:GLU:CG	1:A:40:ASP:N	0.42	2.83	4	1
1:A:49:LEU:HD11	1:A:84:ILE:CG2	0.42	2.44	11	1
1:A:53:PHE:CD1	1:A:53:PHE:C	0.42	2.97	13	1
1:A:13:ARG:CD	1:A:13:ARG:N	0.42	2.83	5	1
1:A:55:TYR:CD2	1:A:85:VAL:HG21	0.42	2.48	18	1
1:A:49:LEU:HD13	1:A:86:LYS:HZ3	0.42	1.71	17	1
1:A:40:ASP:OD1	1:A:40:ASP:C	0.42	2.62	7	1
1:A:14:ILE:HD11	1:A:77:GLU:O	0.42	2.14	11	1
1:A:12:VAL:O	1:A:12:VAL:CG2	0.42	2.68	19	1
1:A:37:THR:C	1:A:39:GLU:N	0.41	2.76	7	1
1:A:41:PHE:CE1	1:A:45:ILE:HG12	0.41	2.49	14	1
1:A:12:VAL:HG13	1:A:78:ASP:N	0.41	2.30	8	1
1:A:55:TYR:CG	1:A:69:LYS:HE3	0.41	2.51	7	1
1:A:55:TYR:CG	1:A:69:LYS:HD2	0.41	2.51	9	1
1:A:22:LEU:C	1:A:22:LEU:CD1	0.41	2.93	13	4
1:A:19:LYS:CG	1:A:19:LYS:O	0.41	2.67	4	1
1:A:11:LEU:HD12	1:A:30:VAL:HG13	0.41	1.91	15	1
1:A:19:LYS:HD2	1:A:19:LYS:C	0.41	2.41	15	1
1:A:39:GLU:HG3	1:A:40:ASP:N	0.41	2.31	15	1
1:A:62:SER:HB2	1:A:77:GLU:CD	0.41	2.41	7	1
1:A:19:LYS:O	1:A:19:LYS:CG	0.41	2.69	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:VAL:HG13	1:A:77:GLU:C	0.41	2.41	12	1
1:A:53:PHE:O	1:A:53:PHE:CD1	0.41	2.74	16	1
1:A:29:VAL:O	1:A:29:VAL:CG1	0.40	2.69	9	2
1:A:59:TRP:CD1	1:A:66:ASN:HB2	0.40	2.51	8	1
1:A:17:LYS:O	1:A:83:GLN:CD	0.40	2.64	10	1
1:A:55:TYR:O	1:A:85:VAL:HG12	0.40	2.17	7	1
1:A:19:LYS:HD3	1:A:19:LYS:C	0.40	2.41	10	1
1:A:46:HIS:C	1:A:48:ASN:N	0.40	2.79	18	1
1:A:55:TYR:O	1:A:85:VAL:HG22	0.40	2.15	6	1
1:A:73:ASP:O	1:A:74:HIS:C	0.40	2.63	15	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	78/93 (84%)	69±2 (89±3%)	8±2 (10±3%)	1±1 (1±1%)	16	66
All	All	1560/1860 (84%)	1386 (89%)	160 (10%)	14 (1%)	16	66

All 6 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	87	LYS	5
1	A	62	SER	3
1	A	20	GLY	2
1	A	34	SER	2
1	A	38	VAL	1
1	A	19	LYS	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	74/84 (88%)	68±2 (92±3%)	6±2 (8±3%)	13	60
All	All	1480/1680 (88%)	1359 (92%)	121 (8%)	13	60

All 32 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	37	THR	20
1	A	22	LEU	11
1	A	66	ASN	10
1	A	19	LYS	8
1	A	41	PHE	7
1	A	72	LYS	6
1	A	64	LYS	6
1	A	30	VAL	5
1	A	78	ASP	4
1	A	24	ASP	4
1	A	87	LYS	4
1	A	61	LEU	4
1	A	51	LYS	3
1	A	48	ASN	3
1	A	85	VAL	2
1	A	83	GLN	2
1	A	11	LEU	2
1	A	45	ILE	2
1	A	73	ASP	2
1	A	12	VAL	2
1	A	47	LYS	2
1	A	52	GLU	2
1	A	44	LYS	1
1	A	86	LYS	1
1	A	79	GLU	1
1	A	69	LYS	1
1	A	80	ASP	1
1	A	16	THR	1
1	A	36	THR	1
1	A	10	LYS	1
1	A	29	VAL	1
1	A	31	LEU	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 oligosaccharides 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

No chemical shift data were provided