



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 06:29 PM BST

PDB ID : 1X0N
Title : NMR structure of growth factor receptor binding protein SH2 domain complexed with the inhibitor
Authors : Ogura, K.; Shiga, T.; Yuzawa, S.; Yokochi, M.; Burke, T.R.; Inagaki, F.
Deposited on : 2005-03-24

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 : 1.7.1 (RC1), CSD as537be (2016)
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

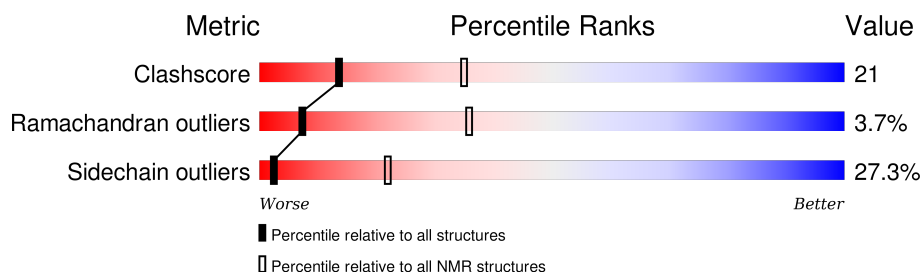
1 Overall quality at a glance

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	104	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 15 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:60-A:153 (94)	0.37	15

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

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

The models can be grouped into 5 clusters and 1 single-model cluster was found.

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

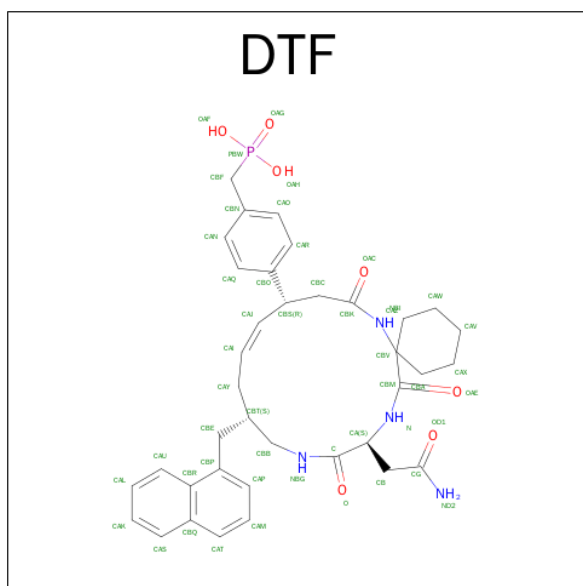
- Molecule 1 is a protein called Growth factor receptor-bound protein 2.

Mol	Chain	Residues	Atoms						Trace
1	A	100	Total	C	H	N	O	S	0
			1628	527	805	147	148	1	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	GLY	-	CLONING ARTIFACT	UNP P62993
A	57	SER	-	CLONING ARTIFACT	UNP P62993

- Molecule 2 is 4-[(10S,14S,18S)-18-(2-AMINO-2-OXOETHYL)-14-(1-NAPHTHYLMETHYL)-8,17,20-TRIOXO-7,16,19-TRIAZASPIRO[5.14]ICOS-11-EN-10-YL]BENZYLPHOSPHONIC ACID (three-letter code: DTF) (formula: C₃₇H₄₅N₄O₇P).



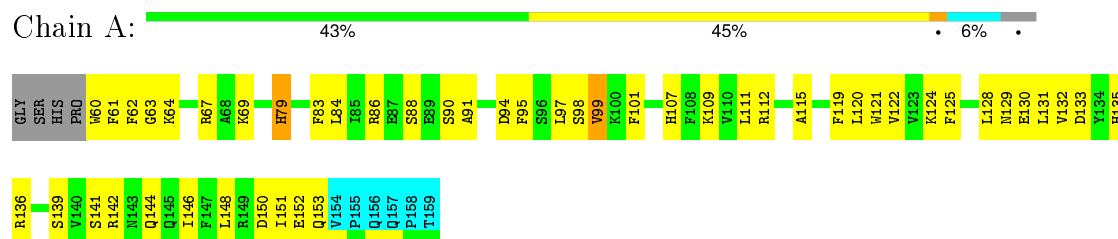
Mol	Chain	Residues	Atoms					
2	A	1	Total	C	H	N	O	P
			92	37	43	4	7	1

4 Residue-property plots

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: Growth factor receptor-bound protein 2

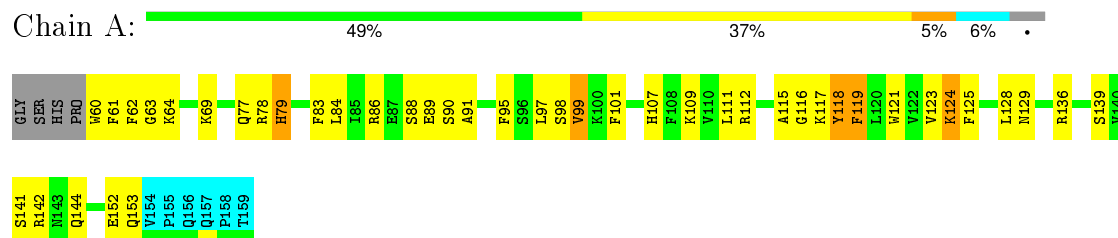


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

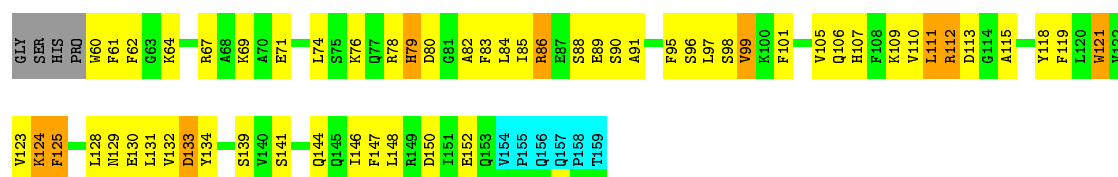
- Molecule 1: Growth factor receptor-bound protein 2



4.2.2 Score per residue for model 2

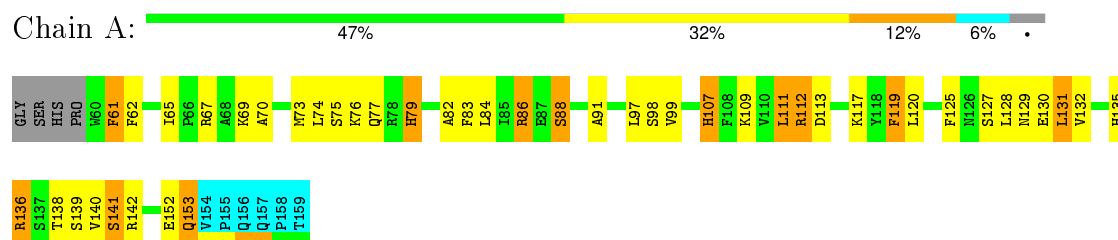
- Molecule 1: Growth factor receptor-bound protein 2





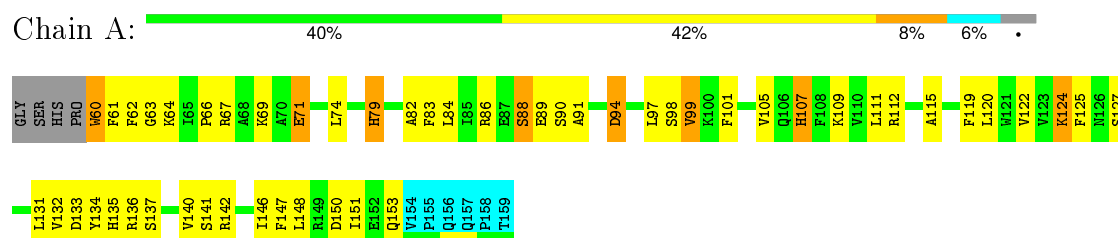
4.2.3 Score per residue for model 3

- Molecule 1: Growth factor receptor-bound protein 2



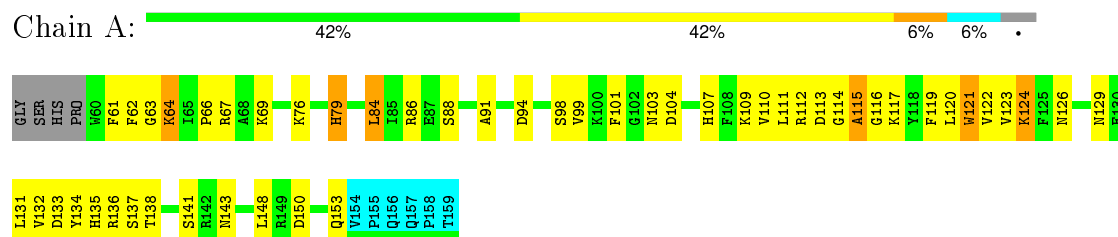
4.2.4 Score per residue for model 4

- Molecule 1: Growth factor receptor-bound protein 2



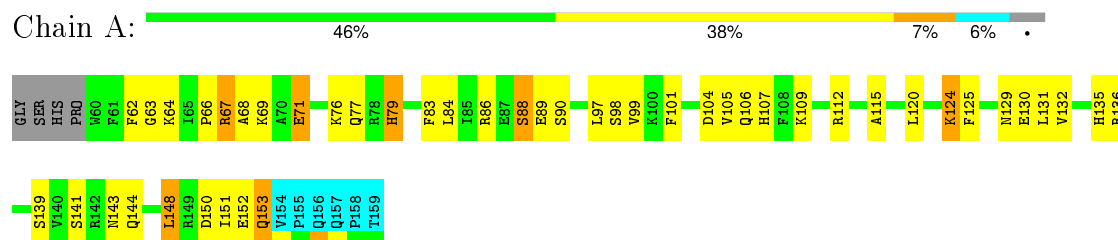
4.2.5 Score per residue for model 5

- Molecule 1: Growth factor receptor-bound protein 2



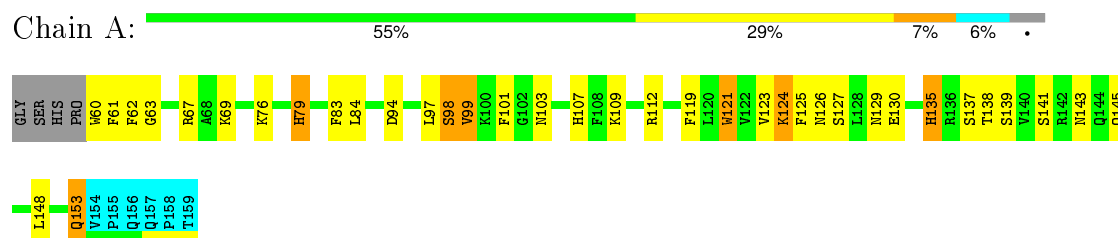
4.2.6 Score per residue for model 6

- Molecule 1: Growth factor receptor-bound protein 2



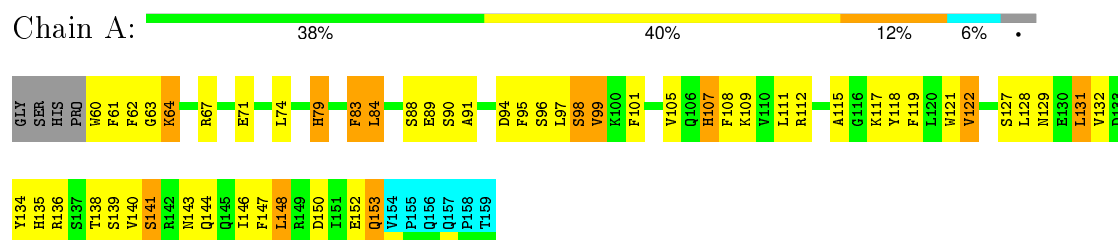
4.2.7 Score per residue for model 7

- Molecule 1: Growth factor receptor-bound protein 2



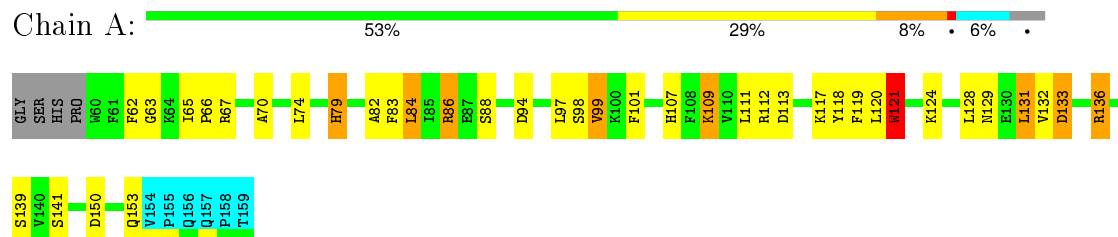
4.2.8 Score per residue for model 8

- Molecule 1: Growth factor receptor-bound protein 2



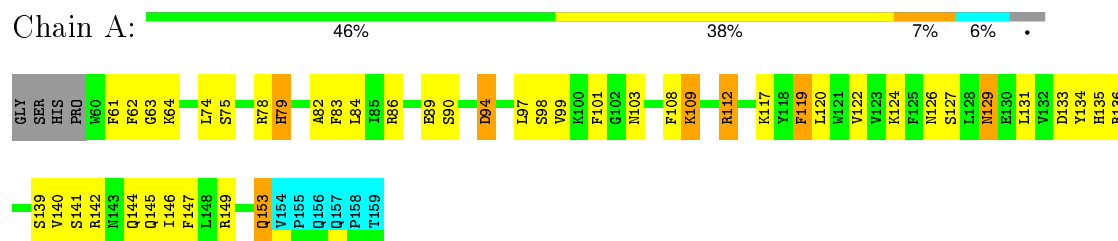
4.2.9 Score per residue for model 9

- Molecule 1: Growth factor receptor-bound protein 2



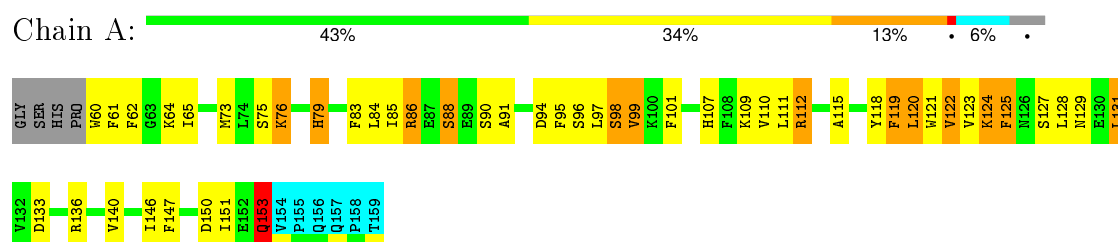
4.2.10 Score per residue for model 10

- Molecule 1: Growth factor receptor-bound protein 2



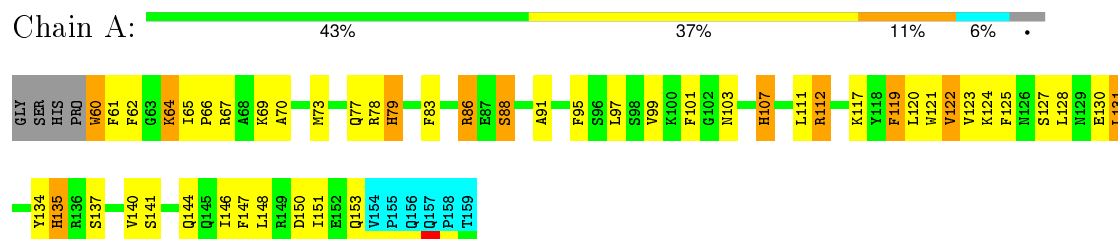
4.2.11 Score per residue for model 11

- Molecule 1: Growth factor receptor-bound protein 2



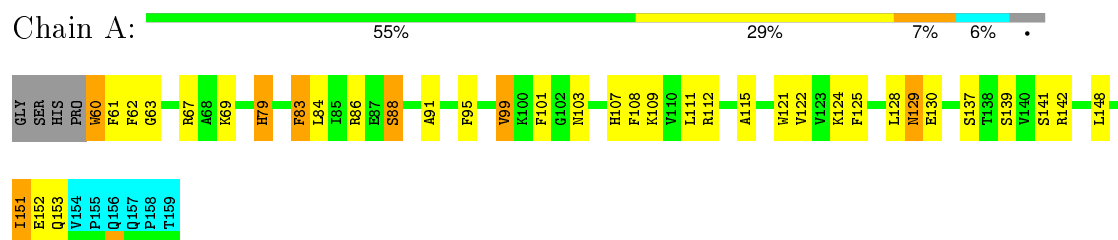
4.2.12 Score per residue for model 12

- Molecule 1: Growth factor receptor-bound protein 2



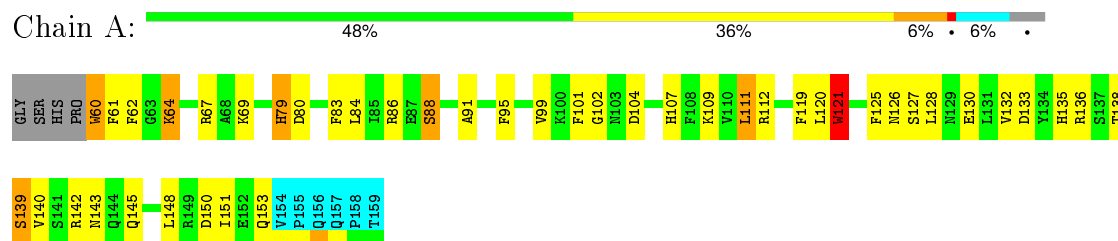
4.2.13 Score per residue for model 13

- Molecule 1: Growth factor receptor-bound protein 2



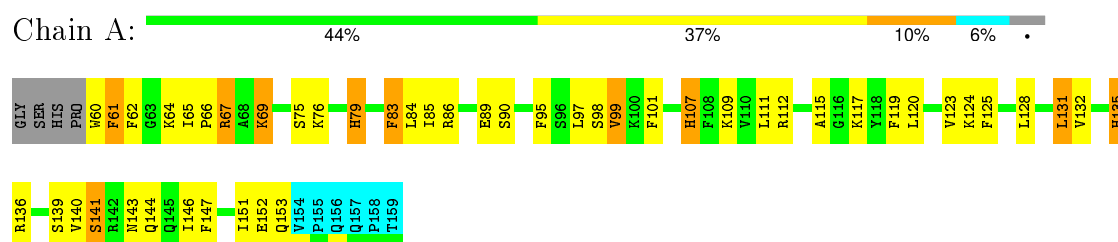
4.2.14 Score per residue for model 14

- Molecule 1: Growth factor receptor-bound protein 2



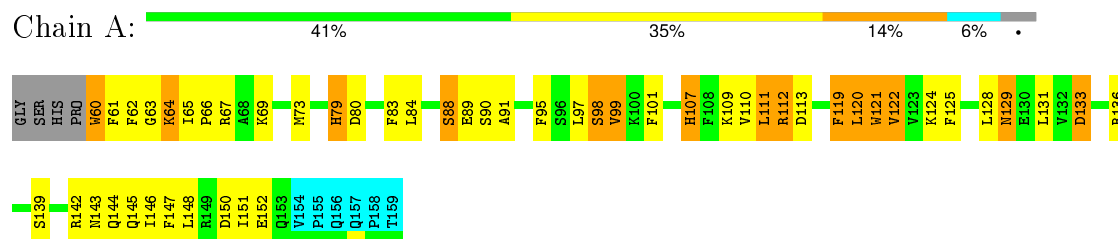
4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Growth factor receptor-bound protein 2



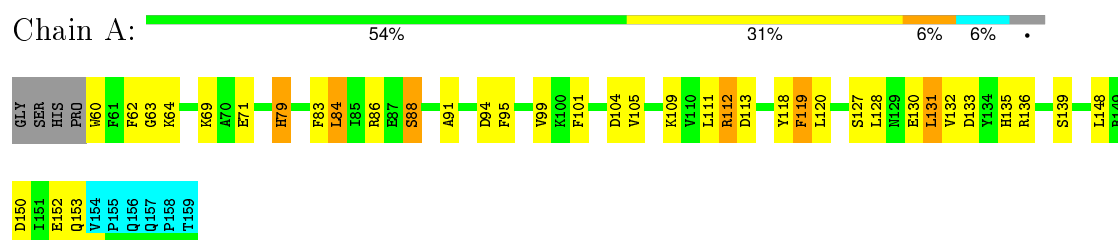
4.2.16 Score per residue for model 16

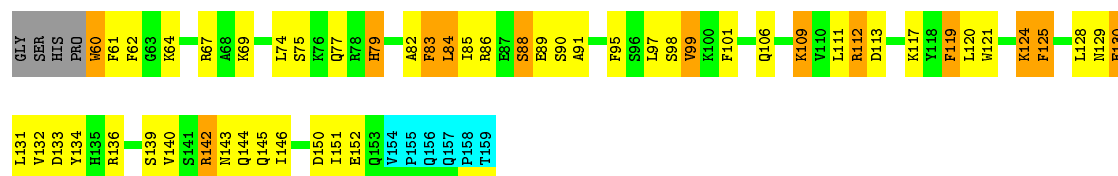
- Molecule 1: Growth factor receptor-bound protein 2



4.2.17 Score per residue for model 17

- Molecule 1: Growth factor receptor-bound protein 2





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 lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	refinement	

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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DTF

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	777	759	758	34±9
2	A	49	43	43	2±2
All	All	16520	16040	16020	680

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:LEU:HD13	1:A:131:LEU:HD21	0.87	1.43	12	1
1:A:60:TRP:CZ2	1:A:132:VAL:HG21	0.86	2.05	15	1
1:A:110:VAL:HG22	1:A:120:LEU:HD11	0.86	1.46	11	3
1:A:120:LEU:HD23	1:A:121:TRP:CD1	0.85	2.06	9	1
1:A:62:PHE:CD1	1:A:84:LEU:HD11	0.83	2.09	16	8
1:A:84:LEU:O	1:A:84:LEU:HD23	0.83	1.72	19	6
1:A:84:LEU:HD23	1:A:84:LEU:O	0.82	1.74	9	11
1:A:60:TRP:CZ2	1:A:132:VAL:HG11	0.82	2.09	20	1
1:A:83:PHE:HB2	1:A:97:LEU:HD21	0.79	1.55	11	12
1:A:95:PHE:CD2	1:A:128:LEU:HD11	0.77	2.15	11	4
1:A:62:PHE:CE1	1:A:84:LEU:HD12	0.76	2.15	13	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:LEU:HD13	1:A:98:SER:N	0.74	1.97	16	12
1:A:88:SER:CB	1:A:91:ALA:HB3	0.74	2.12	13	12
1:A:74:LEU:HD22	1:A:82:ALA:O	0.74	1.81	20	7
1:A:120:LEU:N	1:A:120:LEU:HD13	0.73	1.99	18	1
1:A:97:LEU:HD13	1:A:97:LEU:C	0.72	2.04	15	9
1:A:60:TRP:CZ3	1:A:85:ILE:HD12	0.71	2.21	20	3
1:A:65:ILE:HD12	1:A:65:ILE:O	0.70	1.86	12	1
1:A:88:SER:HB3	1:A:91:ALA:HB3	0.70	1.63	13	7
1:A:84:LEU:C	1:A:84:LEU:HD23	0.70	2.06	20	5
1:A:60:TRP:CZ2	1:A:132:VAL:CG2	0.70	2.74	15	1
1:A:95:PHE:CZ	1:A:128:LEU:HD11	0.69	2.22	16	4
1:A:62:PHE:CD1	1:A:84:LEU:CD1	0.69	2.76	18	9
1:A:95:PHE:CE2	1:A:128:LEU:HD11	0.69	2.23	11	5
1:A:121:TRP:CD1	1:A:121:TRP:N	0.68	2.59	14	1
1:A:60:TRP:CZ2	1:A:132:VAL:CG1	0.68	2.77	20	1
1:A:83:PHE:HB2	1:A:97:LEU:HD11	0.68	1.63	12	3
1:A:97:LEU:C	1:A:97:LEU:HD13	0.67	2.10	2	4
1:A:111:LEU:HD21	2:A:174:DTF:HAT1	0.66	1.65	5	2
1:A:62:PHE:CE1	1:A:153:GLN:NE2	0.66	2.63	5	1
1:A:121:TRP:CH2	2:A:174:DTF:CB	0.65	2.80	14	3
1:A:106:GLN:C	1:A:107:HIS:CD2	0.65	2.70	2	3
1:A:122:VAL:O	1:A:122:VAL:HG23	0.65	1.90	11	1
1:A:125:PHE:CD1	1:A:131:LEU:HD11	0.64	2.27	11	1
1:A:71:GLU:OE1	1:A:105:VAL:HG11	0.64	1.93	18	2
1:A:99:VAL:CG1	1:A:101:PHE:CE2	0.63	2.82	10	12
1:A:62:PHE:CE1	1:A:84:LEU:CD1	0.63	2.82	13	6
1:A:120:LEU:HD22	1:A:120:LEU:O	0.63	1.94	18	1
1:A:111:LEU:HD11	2:A:174:DTF:CAT	0.62	2.23	20	4
1:A:95:PHE:CG	1:A:128:LEU:HD11	0.62	2.30	20	5
1:A:125:PHE:N	1:A:125:PHE:CD1	0.62	2.68	11	2
1:A:135:HIS:ND1	1:A:140:VAL:HG12	0.61	2.09	4	1
1:A:114:GLY:O	1:A:115:ALA:HB2	0.61	1.94	5	2
1:A:60:TRP:CE2	1:A:132:VAL:HG11	0.61	2.30	20	1
1:A:83:PHE:C	1:A:83:PHE:CD1	0.61	2.74	8	3
1:A:135:HIS:CD2	1:A:148:LEU:HD21	0.61	2.31	12	1
1:A:65:ILE:HD11	1:A:84:LEU:HD21	0.60	1.72	15	3
1:A:125:PHE:CE1	1:A:131:LEU:HD21	0.60	2.31	11	1
1:A:99:VAL:HG11	1:A:101:PHE:CE2	0.60	2.31	10	7
1:A:83:PHE:CD1	1:A:83:PHE:C	0.60	2.74	20	4
1:A:125:PHE:HB2	1:A:131:LEU:HD12	0.60	1.71	3	1
1:A:99:VAL:HG11	1:A:101:PHE:CZ	0.60	2.32	2	18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:TRP:N	1:A:151:ILE:CG2	0.60	2.65	4	5
1:A:124:LYS:C	1:A:125:PHE:CD1	0.59	2.75	2	4
1:A:61:PHE:CE1	1:A:62:PHE:O	0.59	2.56	16	6
1:A:83:PHE:CE2	1:A:132:VAL:HG13	0.59	2.33	4	3
1:A:65:ILE:HD11	1:A:86:ARG:HB3	0.59	1.75	3	2
1:A:79:HIS:CE1	1:A:152:GLU:OE2	0.59	2.55	13	1
1:A:124:LYS:O	1:A:125:PHE:CD1	0.59	2.56	16	4
1:A:101:PHE:CE1	1:A:146:ILE:HD13	0.59	2.33	12	1
1:A:84:LEU:HD23	1:A:84:LEU:C	0.58	2.19	6	4
1:A:111:LEU:O	1:A:119:PHE:CD1	0.58	2.57	16	5
1:A:122:VAL:HG22	1:A:122:VAL:O	0.57	1.99	10	1
1:A:120:LEU:CD1	1:A:120:LEU:N	0.57	2.68	18	1
1:A:122:VAL:O	1:A:122:VAL:HG22	0.57	1.98	4	1
1:A:120:LEU:CD1	1:A:131:LEU:CD2	0.57	2.82	15	1
1:A:120:LEU:HD23	1:A:121:TRP:NE1	0.57	2.15	9	1
1:A:123:VAL:HG13	1:A:125:PHE:CZ	0.57	2.35	11	3
1:A:65:ILE:HD11	1:A:86:ARG:CD	0.56	2.30	12	1
1:A:61:PHE:CD1	1:A:62:PHE:N	0.56	2.73	13	15
1:A:111:LEU:HD21	2:A:174:DTF:CAS	0.56	2.30	13	3
1:A:125:PHE:HB2	1:A:131:LEU:HD11	0.56	1.77	19	2
1:A:95:PHE:CD1	1:A:128:LEU:HD11	0.56	2.35	13	7
1:A:70:ALA:HB1	1:A:84:LEU:HD22	0.56	1.77	3	1
1:A:134:TYR:CD1	1:A:134:TYR:C	0.55	2.79	12	3
1:A:135:HIS:CB	1:A:148:LEU:HD11	0.55	2.31	14	1
1:A:120:LEU:HD12	1:A:131:LEU:HD21	0.55	1.78	18	1
1:A:95:PHE:CE1	1:A:128:LEU:HD11	0.55	2.37	16	4
1:A:111:LEU:HD21	2:A:174:DTF:HAS1	0.55	1.77	3	1
1:A:107:HIS:N	1:A:107:HIS:CD2	0.54	2.75	8	2
1:A:111:LEU:HD11	2:A:174:DTF:CAS	0.54	2.31	3	1
1:A:97:LEU:C	1:A:97:LEU:CD1	0.54	2.75	15	5
1:A:83:PHE:CZ	1:A:132:VAL:HG11	0.54	2.38	6	4
1:A:111:LEU:HD21	2:A:174:DTF:CAT	0.54	2.32	5	1
1:A:83:PHE:CE2	1:A:132:VAL:CG1	0.54	2.90	8	4
1:A:71:GLU:OE2	1:A:107:HIS:CE1	0.54	2.61	6	1
1:A:79:HIS:CD2	1:A:79:HIS:N	0.54	2.76	16	10
1:A:65:ILE:CD1	1:A:70:ALA:HB2	0.53	2.34	9	2
1:A:107:HIS:CD2	1:A:107:HIS:N	0.53	2.74	12	4
1:A:135:HIS:NE2	1:A:140:VAL:HG23	0.53	2.18	10	1
1:A:119:PHE:O	1:A:120:LEU:HD12	0.53	2.04	5	1
1:A:135:HIS:HB3	1:A:148:LEU:HD11	0.53	1.80	17	4
1:A:121:TRP:C	1:A:122:VAL:HG23	0.53	2.24	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:HIS:N	1:A:79:HIS:CD2	0.52	2.78	14	9
1:A:119:PHE:CD1	1:A:119:PHE:N	0.52	2.78	10	3
1:A:71:GLU:N	1:A:71:GLU:OE1	0.52	2.43	6	2
1:A:97:LEU:CD1	1:A:97:LEU:C	0.52	2.77	11	6
1:A:140:VAL:HG13	1:A:141:SER:N	0.52	2.20	3	1
1:A:99:VAL:HG12	1:A:101:PHE:CE2	0.52	2.40	18	4
1:A:111:LEU:HB3	1:A:119:PHE:CE2	0.51	2.40	18	1
1:A:121:TRP:CZ2	1:A:142:ARG:HD2	0.51	2.40	20	1
1:A:123:VAL:HG22	1:A:124:LYS:H	0.51	1.66	5	2
1:A:83:PHE:CZ	1:A:132:VAL:CG1	0.51	2.94	6	5
1:A:112:ARG:HG2	1:A:118:TYR:CD1	0.51	2.41	2	3
1:A:129:ASN:ND2	1:A:129:ASN:C	0.51	2.64	10	3
1:A:111:LEU:HB3	1:A:119:PHE:CE1	0.51	2.40	4	3
1:A:121:TRP:O	1:A:122:VAL:C	0.51	2.49	11	2
1:A:129:ASN:ND2	1:A:130:GLU:N	0.51	2.59	13	1
1:A:111:LEU:HD21	2:A:174:DTF:CBQ	0.51	2.36	2	1
1:A:84:LEU:C	1:A:84:LEU:CD2	0.50	2.78	20	1
1:A:112:ARG:HA	1:A:119:PHE:CE1	0.50	2.41	20	1
1:A:135:HIS:ND1	1:A:140:VAL:CG1	0.50	2.74	4	1
1:A:121:TRP:O	1:A:123:VAL:N	0.50	2.44	12	2
1:A:60:TRP:CE2	1:A:132:VAL:HG21	0.50	2.40	15	1
1:A:120:LEU:HD22	1:A:120:LEU:C	0.50	2.26	18	1
1:A:119:PHE:C	1:A:120:LEU:HD12	0.50	2.27	12	2
1:A:135:HIS:NE2	1:A:140:VAL:HG22	0.50	2.22	12	1
1:A:126:ASN:CG	1:A:127:SER:N	0.50	2.65	7	1
1:A:111:LEU:O	1:A:119:PHE:CE1	0.50	2.65	11	2
1:A:73:MET:O	1:A:77:GLN:NE2	0.50	2.45	12	2
1:A:83:PHE:CD1	1:A:149:ARG:O	0.50	2.64	10	1
1:A:112:ARG:CA	1:A:119:PHE:CE1	0.50	2.94	20	2
1:A:125:PHE:CD1	1:A:125:PHE:N	0.50	2.80	2	2
1:A:121:TRP:CZ2	2:A:174:DTF:HB1	0.50	2.42	12	7
1:A:93:GLY:O	1:A:112:ARG:NE	0.50	2.45	18	1
1:A:111:LEU:HD11	2:A:174:DTF:CBQ	0.50	2.37	3	1
1:A:120:LEU:CB	1:A:121:TRP:CD1	0.49	2.95	14	1
1:A:146:ILE:HG22	1:A:147:PHE:N	0.49	2.22	12	10
1:A:118:TYR:HB2	1:A:131:LEU:HD13	0.49	1.83	8	1
1:A:133:ASP:O	1:A:136:ARG:N	0.49	2.45	20	5
1:A:123:VAL:HG22	1:A:124:LYS:N	0.49	2.23	2	2
1:A:71:GLU:OE1	1:A:71:GLU:N	0.49	2.45	4	1
1:A:71:GLU:O	1:A:75:SER:CB	0.49	2.60	19	1
1:A:120:LEU:O	1:A:122:VAL:N	0.49	2.45	18	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:GLY:O	1:A:118:TYR:CE1	0.49	2.65	1	1
1:A:95:PHE:CE1	1:A:128:LEU:CD1	0.48	2.96	15	2
1:A:114:GLY:O	1:A:115:ALA:CB	0.48	2.59	5	2
1:A:135:HIS:CE1	1:A:140:VAL:HG23	0.48	2.42	10	1
1:A:152:GLU:CG	1:A:152:GLU:O	0.48	2.60	17	1
1:A:111:LEU:HD11	2:A:174:DTF:HAS1	0.48	1.85	2	1
1:A:121:TRP:N	1:A:121:TRP:CD1	0.48	2.78	2	2
1:A:83:PHE:CD2	1:A:148:LEU:HD23	0.48	2.43	6	2
1:A:120:LEU:HD12	1:A:131:LEU:CD2	0.48	2.39	18	1
1:A:135:HIS:CB	1:A:148:LEU:CD1	0.48	2.92	14	1
1:A:95:PHE:CD1	1:A:128:LEU:CD1	0.48	2.97	20	1
1:A:121:TRP:CD1	1:A:122:VAL:HG13	0.48	2.42	5	1
1:A:146:ILE:CG2	1:A:147:PHE:N	0.48	2.77	8	6
1:A:83:PHE:CE2	1:A:132:VAL:HG11	0.48	2.43	19	2
1:A:124:LYS:C	1:A:125:PHE:CG	0.48	2.87	2	5
1:A:74:LEU:HD23	1:A:151:ILE:HG13	0.48	1.84	18	1
1:A:140:VAL:O	1:A:140:VAL:HG22	0.48	2.08	14	1
1:A:135:HIS:CG	1:A:140:VAL:CG1	0.48	2.96	4	1
1:A:74:LEU:HD11	1:A:98:SER:OG	0.48	2.09	8	1
1:A:119:PHE:CB	1:A:123:VAL:O	0.48	2.62	1	1
1:A:71:GLU:HG2	1:A:105:VAL:HG11	0.48	1.86	8	3
1:A:99:VAL:HG21	1:A:148:LEU:HD22	0.48	1.85	14	1
1:A:111:LEU:HB3	1:A:119:PHE:CZ	0.47	2.44	4	5
1:A:108:PHE:CE1	2:A:174:DTF:CBA	0.47	2.97	13	1
1:A:135:HIS:CD2	1:A:140:VAL:HG12	0.47	2.43	15	1
1:A:140:VAL:HG22	1:A:146:ILE:O	0.47	2.09	11	1
1:A:71:GLU:CA	1:A:71:GLU:OE1	0.47	2.62	18	1
1:A:111:LEU:CD1	2:A:174:DTF:CAT	0.47	2.91	20	1
1:A:66:PRO:O	1:A:69:LYS:N	0.47	2.47	15	3
1:A:125:PHE:CG	1:A:131:LEU:CD1	0.47	2.97	11	2
1:A:132:VAL:O	1:A:136:ARG:CB	0.47	2.62	3	1
1:A:97:LEU:HD23	1:A:108:PHE:CD2	0.47	2.45	10	1
1:A:125:PHE:CD1	1:A:130:GLU:HB3	0.47	2.45	12	1
1:A:112:ARG:HG2	1:A:118:TYR:CD2	0.47	2.45	11	1
1:A:62:PHE:CD1	1:A:84:LEU:HD12	0.47	2.44	5	1
1:A:65:ILE:HD13	1:A:70:ALA:HB2	0.47	1.86	12	1
1:A:66:PRO:O	1:A:67:ARG:C	0.47	2.53	12	9
1:A:71:GLU:OE2	1:A:105:VAL:CG1	0.47	2.63	6	1
1:A:128:LEU:O	1:A:131:LEU:N	0.47	2.48	9	3
1:A:93:GLY:O	1:A:112:ARG:CZ	0.47	2.63	18	1
1:A:121:TRP:CH2	2:A:174:DTF:HB1	0.47	2.44	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:PHE:CD2	1:A:130:GLU:HB3	0.46	2.45	20	1
1:A:60:TRP:CG	1:A:83:PHE:CE1	0.46	3.03	11	2
1:A:140:VAL:HG11	1:A:148:LEU:CD2	0.46	2.39	14	1
1:A:107:HIS:C	1:A:108:PHE:CD1	0.46	2.89	8	1
1:A:125:PHE:CG	1:A:130:GLU:HB3	0.46	2.46	14	2
1:A:60:TRP:HA	1:A:83:PHE:CE1	0.46	2.45	13	1
1:A:83:PHE:CD2	1:A:148:LEU:CD2	0.46	2.99	8	1
1:A:111:LEU:C	1:A:119:PHE:CE1	0.46	2.89	20	3
1:A:120:LEU:HB3	1:A:121:TRP:CD1	0.46	2.44	14	1
1:A:129:ASN:C	1:A:129:ASN:ND2	0.46	2.68	16	1
1:A:60:TRP:CB	1:A:83:PHE:CE1	0.46	2.98	2	1
1:A:60:TRP:CH2	1:A:85:ILE:HD12	0.46	2.46	20	1
1:A:135:HIS:CE1	1:A:140:VAL:HG12	0.46	2.46	4	1
1:A:125:PHE:CG	1:A:131:LEU:HD11	0.46	2.45	11	2
1:A:120:LEU:CD1	1:A:131:LEU:HD22	0.46	2.40	15	1
1:A:67:ARG:NH1	1:A:107:HIS:NE2	0.45	2.64	2	1
1:A:119:PHE:N	1:A:119:PHE:CD1	0.45	2.85	14	3
1:A:84:LEU:CD2	1:A:84:LEU:O	0.45	2.60	7	3
1:A:109:LYS:O	1:A:120:LEU:HD12	0.45	2.11	9	1
1:A:120:LEU:CD2	1:A:121:TRP:CD1	0.45	2.90	9	1
1:A:123:VAL:CG2	1:A:125:PHE:CE2	0.45	3.00	7	1
1:A:125:PHE:CE1	1:A:130:GLU:OE1	0.45	2.70	13	1
1:A:71:GLU:OE2	1:A:107:HIS:NE2	0.45	2.50	18	2
1:A:109:LYS:HG2	2:A:174:DTF:CAR	0.45	2.40	10	1
1:A:60:TRP:HA	1:A:83:PHE:CZ	0.45	2.47	13	1
1:A:67:ARG:NH2	2:A:174:DTF:OAG	0.45	2.50	12	3
1:A:86:ARG:CZ	2:A:174:DTF:OAF	0.45	2.65	9	1
1:A:128:LEU:O	1:A:132:VAL:HG23	0.45	2.12	17	1
1:A:97:LEU:O	1:A:107:HIS:CB	0.45	2.64	12	2
1:A:110:VAL:O	1:A:112:ARG:NH2	0.45	2.50	2	1
1:A:145:GLN:O	1:A:145:GLN:CG	0.45	2.64	10	1
1:A:62:PHE:CE1	1:A:84:LEU:HD11	0.45	2.46	16	1
1:A:97:LEU:HD11	1:A:99:VAL:HG23	0.44	1.90	2	3
1:A:99:VAL:CG2	1:A:148:LEU:HD22	0.44	2.42	18	1
1:A:86:ARG:NH2	2:A:174:DTF:OAF	0.44	2.50	2	3
1:A:60:TRP:CB	1:A:83:PHE:CE2	0.44	3.00	7	2
1:A:70:ALA:CB	1:A:84:LEU:HD22	0.44	2.41	3	1
1:A:122:VAL:O	1:A:122:VAL:CG2	0.44	2.62	11	1
1:A:67:ARG:NH2	2:A:174:DTF:OAH	0.44	2.50	2	1
1:A:129:ASN:HD22	1:A:130:GLU:N	0.44	2.10	13	1
1:A:101:PHE:CE1	1:A:141:SER:HB3	0.44	2.47	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:ASN:C	1:A:129:ASN:OD1	0.44	2.56	3	1
1:A:129:ASN:O	1:A:132:VAL:HG22	0.44	2.12	5	1
1:A:107:HIS:CD2	2:A:174:DTF:HBC2	0.44	2.48	15	2
1:A:60:TRP:N	1:A:151:ILE:HG22	0.44	2.27	18	2
1:A:107:HIS:CD2	2:A:174:DTF:CBO	0.44	3.00	1	1
1:A:71:GLU:HG2	1:A:105:VAL:CG1	0.44	2.43	19	1
1:A:84:LEU:CD2	1:A:84:LEU:C	0.44	2.86	7	1
1:A:124:LYS:O	1:A:125:PHE:CG	0.43	2.71	6	1
1:A:135:HIS:HA	1:A:138:THR:HG22	0.43	1.90	8	2
1:A:125:PHE:CD1	1:A:130:GLU:OE1	0.43	2.72	7	1
1:A:73:MET:O	1:A:76:LYS:CG	0.43	2.66	11	1
1:A:121:TRP:O	1:A:122:VAL:CB	0.43	2.67	8	1
1:A:121:TRP:CZ2	2:A:174:DTF:CB	0.43	3.01	13	2
1:A:112:ARG:HA	1:A:119:PHE:CZ	0.43	2.48	12	2
1:A:135:HIS:CG	1:A:148:LEU:HG	0.43	2.49	12	1
1:A:60:TRP:HB2	1:A:83:PHE:CE1	0.43	2.48	2	2
1:A:120:LEU:HB3	1:A:121:TRP:NE1	0.43	2.28	14	1
1:A:152:GLU:O	1:A:152:GLU:CG	0.43	2.65	1	1
1:A:60:TRP:CG	1:A:83:PHE:CZ	0.43	3.06	8	1
1:A:123:VAL:HG22	1:A:125:PHE:CZ	0.43	2.49	15	1
1:A:85:ILE:HG22	1:A:95:PHE:CD1	0.43	2.49	11	1
1:A:134:TYR:C	1:A:134:TYR:CD1	0.43	2.92	4	2
1:A:62:PHE:CZ	1:A:73:MET:HG3	0.43	2.49	16	1
1:A:65:ILE:CD1	1:A:65:ILE:O	0.43	2.65	12	1
1:A:128:LEU:HA	1:A:131:LEU:HD21	0.43	1.90	17	1
1:A:106:GLN:OE1	2:A:174:DTF:CAV	0.43	2.66	20	1
1:A:95:PHE:CE2	1:A:128:LEU:CD1	0.43	2.97	11	1
1:A:71:GLU:OE1	1:A:105:VAL:CG1	0.43	2.66	18	1
1:A:83:PHE:CB	1:A:97:LEU:HD21	0.42	2.35	8	1
1:A:135:HIS:CG	1:A:140:VAL:HG12	0.42	2.49	15	1
1:A:125:PHE:CE1	1:A:131:LEU:CD2	0.42	3.02	11	1
1:A:152:GLU:O	1:A:153:GLN:C	0.42	2.56	3	2
1:A:123:VAL:CG2	1:A:125:PHE:CZ	0.42	3.02	15	1
1:A:99:VAL:HG21	1:A:148:LEU:CD1	0.42	2.44	4	1
1:A:94:ASP:OD1	1:A:112:ARG:NH2	0.42	2.52	4	2
1:A:136:ARG:NH1	1:A:148:LEU:O	0.42	2.52	5	1
1:A:66:PRO:O	1:A:68:ALA:N	0.42	2.53	6	1
1:A:140:VAL:HG23	1:A:141:SER:N	0.42	2.30	15	2
1:A:127:SER:O	1:A:131:LEU:HD12	0.42	2.15	11	1
1:A:125:PHE:CD2	1:A:131:LEU:HG	0.42	2.49	11	1
1:A:130:GLU:O	1:A:134:TYR:CB	0.42	2.68	20	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:TRP:HB3	1:A:151:ILE:HG22	0.42	1.90	16	1
1:A:125:PHE:CE2	1:A:131:LEU:HG	0.42	2.48	11	1
1:A:107:HIS:CD2	2:A:174:DTF:CAR	0.42	3.03	1	1
1:A:125:PHE:HD2	1:A:131:LEU:HD12	0.42	1.73	6	1
1:A:109:LYS:O	1:A:111:LEU:CD2	0.42	2.68	20	1
1:A:77:GLN:NE2	1:A:151:ILE:HG12	0.42	2.30	12	3
1:A:120:LEU:CD2	1:A:120:LEU:C	0.42	2.88	18	1
1:A:133:ASP:O	1:A:134:TYR:C	0.42	2.58	2	2
1:A:108:PHE:CD1	2:A:174:DTF:HBA2	0.42	2.50	13	1
1:A:121:TRP:CZ3	2:A:174:DTF:HA1	0.42	2.50	14	1
1:A:129:ASN:O	1:A:132:VAL:CG2	0.42	2.68	9	1
1:A:60:TRP:CG	1:A:83:PHE:CE2	0.41	3.08	7	2
1:A:63:GLY:O	1:A:64:LYS:C	0.41	2.57	16	1
1:A:111:LEU:HD22	1:A:111:LEU:N	0.41	2.30	1	1
1:A:120:LEU:CD1	1:A:131:LEU:HD21	0.41	2.30	12	1
1:A:135:HIS:CD2	1:A:148:LEU:CD2	0.41	3.03	12	1
1:A:111:LEU:CD2	2:A:174:DTF:CAS	0.41	2.98	12	1
1:A:99:VAL:HG21	1:A:148:LEU:CD2	0.41	2.45	18	2
1:A:121:TRP:CH2	2:A:174:DTF:HA1	0.41	2.51	14	2
1:A:111:LEU:N	1:A:111:LEU:HD22	0.41	2.30	20	1
1:A:112:ARG:N	1:A:119:PHE:CE1	0.41	2.88	20	1
1:A:101:PHE:CE1	1:A:146:ILE:HD12	0.41	2.50	20	1
1:A:122:VAL:CG2	1:A:122:VAL:O	0.41	2.68	10	2
1:A:85:ILE:CG2	1:A:95:PHE:CD1	0.41	3.03	11	1
1:A:112:ARG:C	1:A:119:PHE:CZ	0.41	2.94	16	1
1:A:121:TRP:C	1:A:123:VAL:N	0.41	2.74	12	1
1:A:128:LEU:O	1:A:129:ASN:C	0.41	2.59	9	2
1:A:135:HIS:O	1:A:138:THR:O	0.41	2.39	14	1
1:A:134:TYR:O	1:A:138:THR:HG22	0.41	2.16	5	1
1:A:83:PHE:CE1	1:A:149:ARG:O	0.41	2.74	10	1
1:A:111:LEU:HG	2:A:174:DTF:CAS	0.41	2.46	17	1
1:A:97:LEU:HG	1:A:98:SER:N	0.40	2.31	10	1
1:A:79:HIS:H	1:A:79:HIS:CD2	0.40	2.33	14	1
1:A:63:GLY:O	1:A:64:LYS:O	0.40	2.39	16	1
1:A:119:PHE:HB3	1:A:124:LYS:CB	0.40	2.46	7	1
1:A:62:PHE:CZ	1:A:84:LEU:HD12	0.40	2.51	13	1
1:A:60:TRP:HB2	1:A:83:PHE:CE2	0.40	2.51	17	1
1:A:118:TYR:CD1	1:A:118:TYR:N	0.40	2.89	1	1
1:A:60:TRP:N	1:A:153:GLN:OE1	0.40	2.55	12	1
1:A:95:PHE:CZ	1:A:128:LEU:CD1	0.40	3.02	16	1
1:A:83:PHE:CZ	1:A:132:VAL:HG13	0.40	2.51	2	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	93/104 (89%)	78±2 (84±2%)	12±2 (12±3%)	3±1 (4±1%)	7	36
All	All	1860/2080 (89%)	1561 (84%)	231 (12%)	68 (4%)	7	36

All 14 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	139	SER	16
1	A	63	GLY	12
1	A	115	ALA	10
1	A	64	LYS	8
1	A	121	TRP	5
1	A	153	GLN	5
1	A	122	VAL	4
1	A	88	SER	2
1	A	79	HIS	1
1	A	116	GLY	1
1	A	67	ARG	1
1	A	77	GLN	1
1	A	102	GLY	1
1	A	140	VAL	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	83/92 (90%)	60±3 (73±3%)	23±3 (27±3%)	2	22
All	All	1660/1840 (90%)	1206 (73%)	454 (27%)	2	22

All 58 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	79	HIS	20
1	A	109	LYS	19
1	A	112	ARG	18
1	A	86	ARG	16
1	A	124	LYS	14
1	A	141	SER	13
1	A	107	HIS	13
1	A	69	LYS	13
1	A	131	LEU	12
1	A	150	ASP	12
1	A	99	VAL	12
1	A	90	SER	12
1	A	144	GLN	11
1	A	88	SER	11
1	A	136	ARG	11
1	A	64	LYS	11
1	A	129	ASN	11
1	A	89	GLU	10
1	A	119	PHE	10
1	A	117	LYS	10
1	A	94	ASP	10
1	A	113	ASP	9
1	A	120	LEU	9
1	A	142	ARG	9
1	A	153	GLN	9
1	A	127	SER	8
1	A	143	ASN	8
1	A	98	SER	8
1	A	76	LYS	8
1	A	60	TRP	7
1	A	84	LEU	7
1	A	133	ASP	7
1	A	103	ASN	6
1	A	152	GLU	6
1	A	67	ARG	6
1	A	130	GLU	6
1	A	121	TRP	5
1	A	137	SER	5
1	A	75	SER	5
1	A	78	ARG	5
1	A	111	LEU	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	148	LEU	4
1	A	104	ASP	4
1	A	83	PHE	4
1	A	151	ILE	4
1	A	125	PHE	4
1	A	135	HIS	4
1	A	145	GLN	4
1	A	126	ASN	3
1	A	71	GLU	3
1	A	80	ASP	3
1	A	96	SER	3
1	A	122	VAL	2
1	A	61	PHE	2
1	A	138	THR	1
1	A	139	SER	1
1	A	118	TYR	1
1	A	105	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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	DTF	A	174	-	51,53,53	1.46±0.00	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	DTF	A	174	-	67,75,75	1.23±0.00	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTF	A	174	-	-	0±0,51,61,61	0±0,4,5,5

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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