



Full wwPDB NMR Structure Validation Report ⓘ

Mar 29, 2026 – 04:24 PM UTC

PDB ID : 1X0N / pdb_00001x0n
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

<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
Mogul	:	2022.3.0, CSD as543be (2022)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

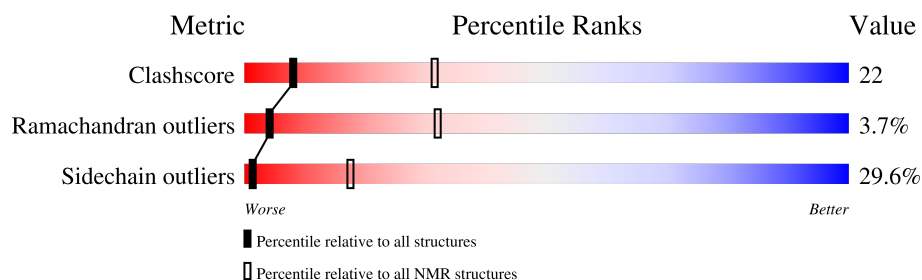
1 Overall quality at a glance

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	104	36% 52% 6%

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)	0.64	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

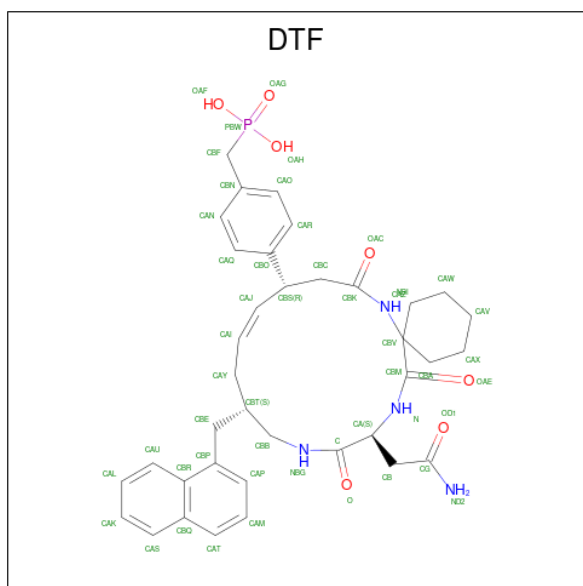
- Molecule 1 is a protein called Growth factor receptor-bound protein 2.

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 (CCD ID: DTF) (formula: $C_{37}H_{45}N_4O_7P$).



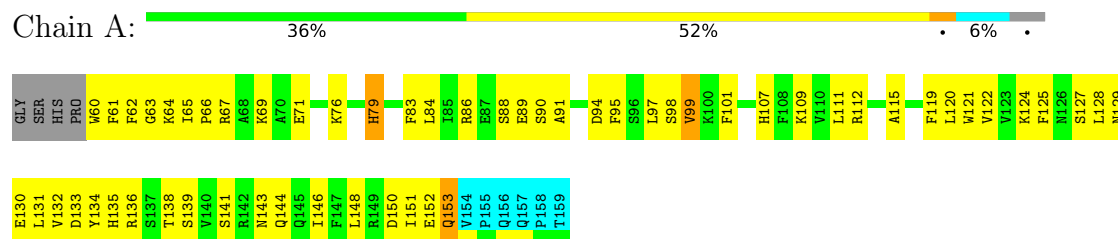
Mol	Chain	Residues	Atoms					
2	A	1	Total	C	H	N	O	P
			92	37	43	4	7	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, 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: Growth factor receptor-bound protein 2

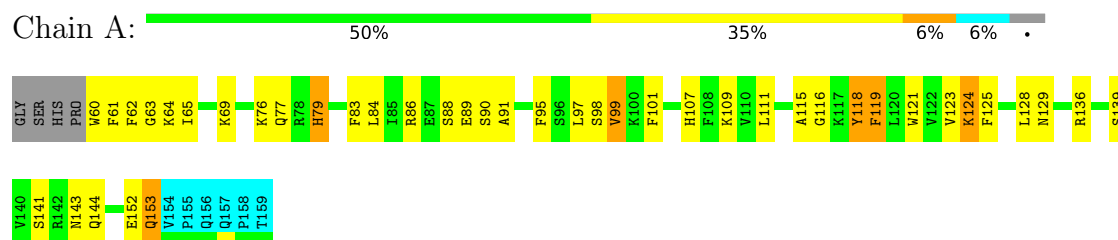


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

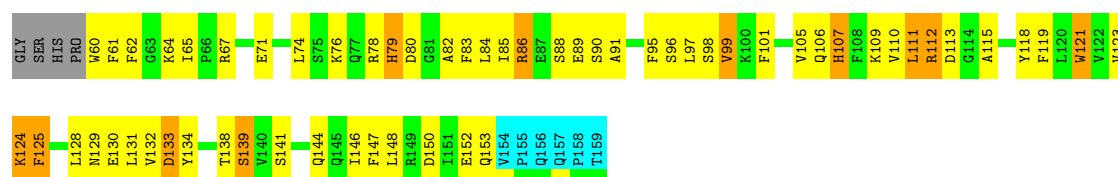
- Molecule 1: Growth factor receptor-bound protein 2



4.2.2 Score per residue for model 2

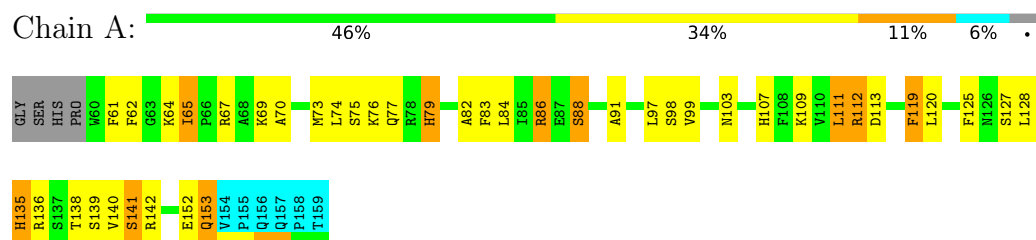
- Molecule 1: Growth factor receptor-bound protein 2





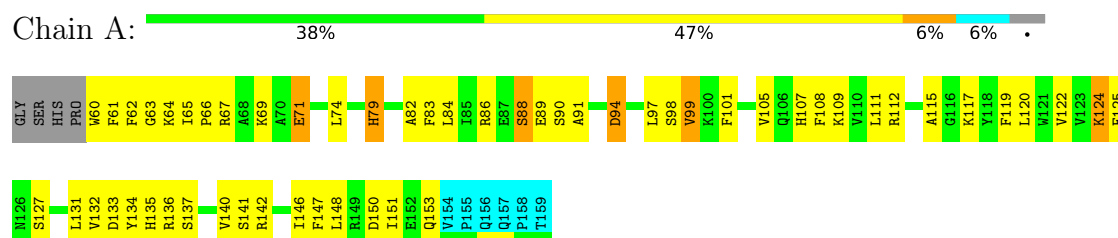
4.2.3 Score per residue for model 3

- Molecule 1: Growth factor receptor-bound protein 2



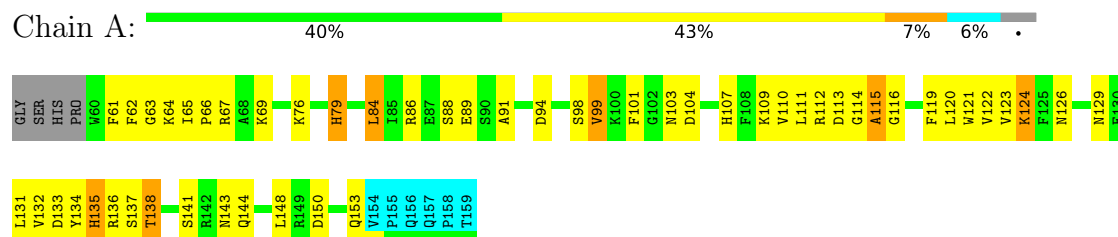
4.2.4 Score per residue for model 4

- Molecule 1: Growth factor receptor-bound protein 2



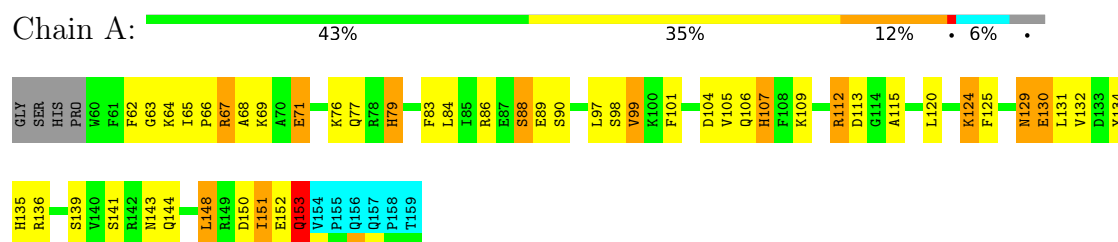
4.2.5 Score per residue for model 5

- Molecule 1: Growth factor receptor-bound protein 2



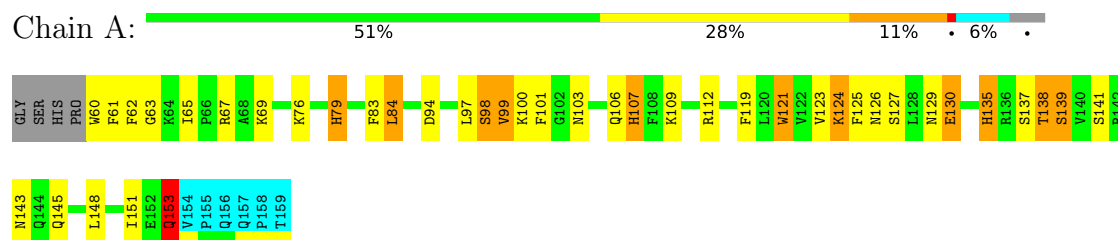
4.2.6 Score per residue for model 6

- Molecule 1: Growth factor receptor-bound protein 2



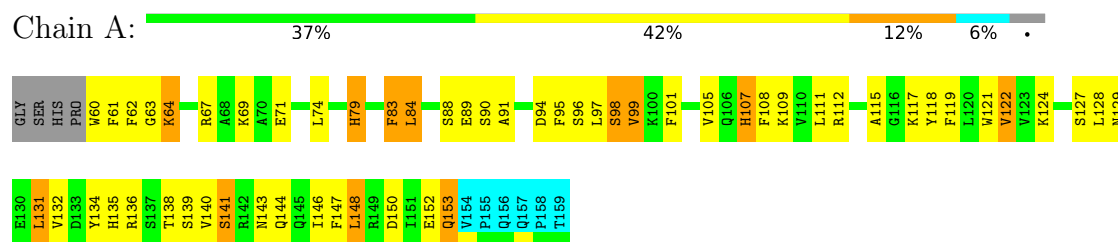
4.2.7 Score per residue for model 7

- Molecule 1: Growth factor receptor-bound protein 2



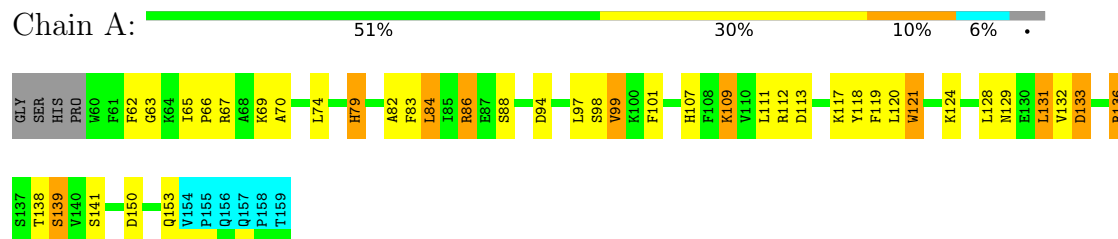
4.2.8 Score per residue for model 8

- Molecule 1: Growth factor receptor-bound protein 2



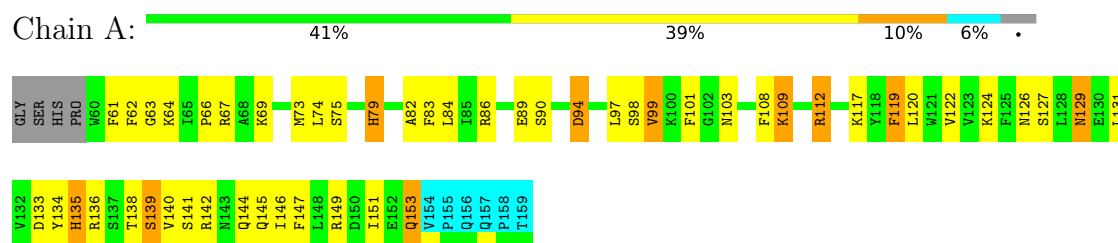
4.2.9 Score per residue for model 9

- Molecule 1: Growth factor receptor-bound protein 2



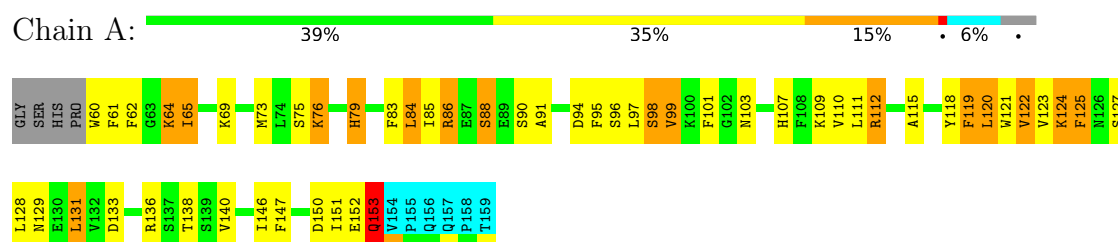
4.2.10 Score per residue for model 10

- Molecule 1: Growth factor receptor-bound protein 2



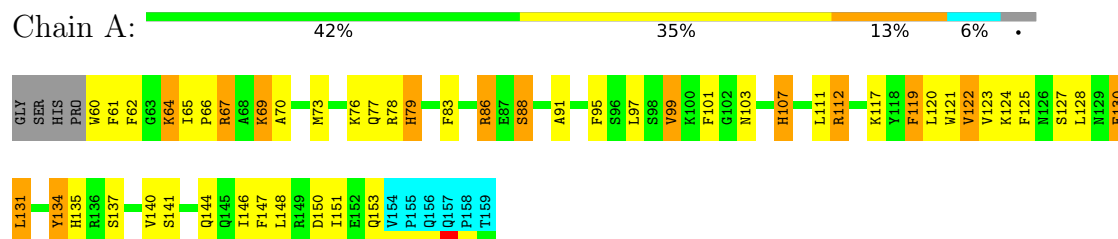
4.2.11 Score per residue for model 11

- Molecule 1: Growth factor receptor-bound protein 2



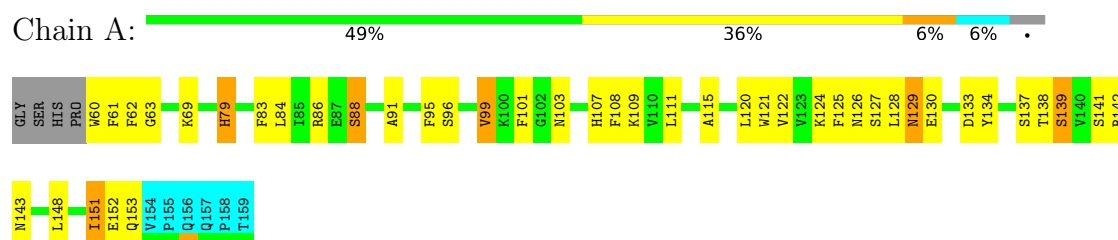
4.2.12 Score per residue for model 12

- Molecule 1: Growth factor receptor-bound protein 2



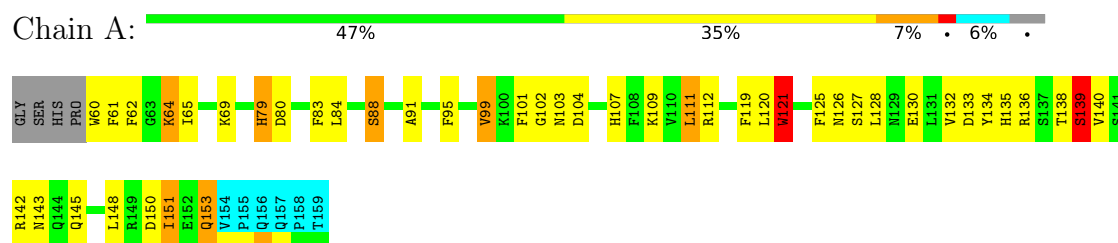
4.2.13 Score per residue for model 13

- Molecule 1: Growth factor receptor-bound protein 2



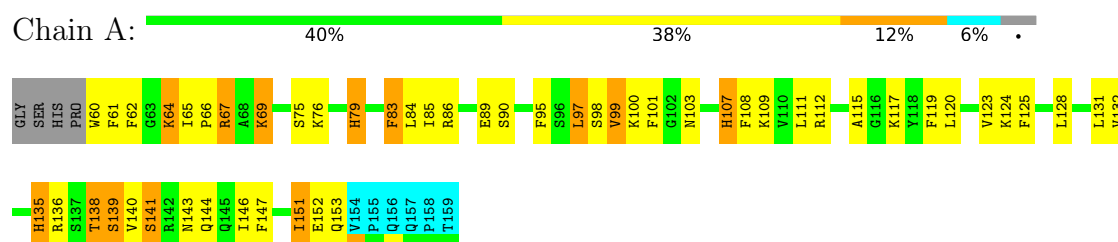
4.2.14 Score per residue for model 14

- Molecule 1: Growth factor receptor-bound protein 2



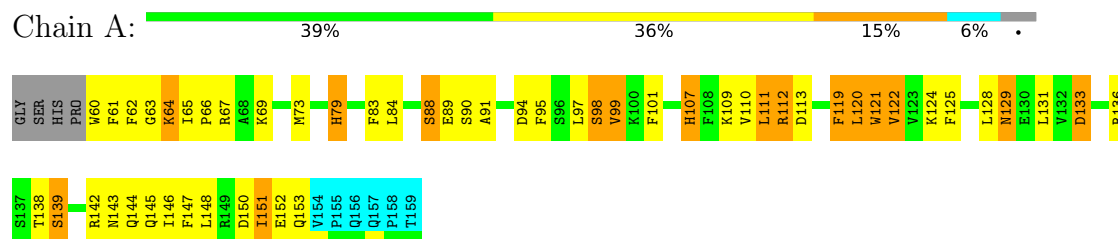
4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Growth factor receptor-bound protein 2



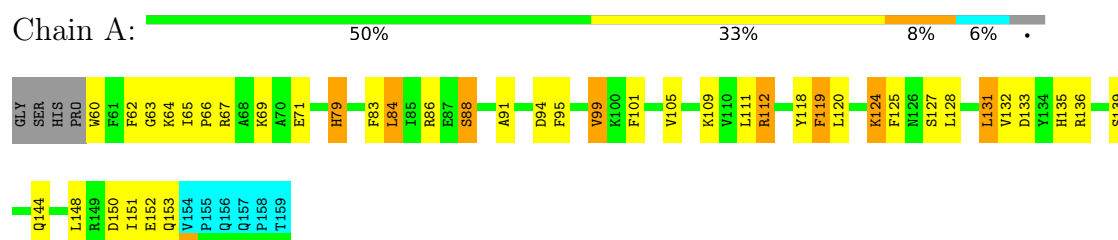
4.2.16 Score per residue for model 16

- Molecule 1: Growth factor receptor-bound protein 2



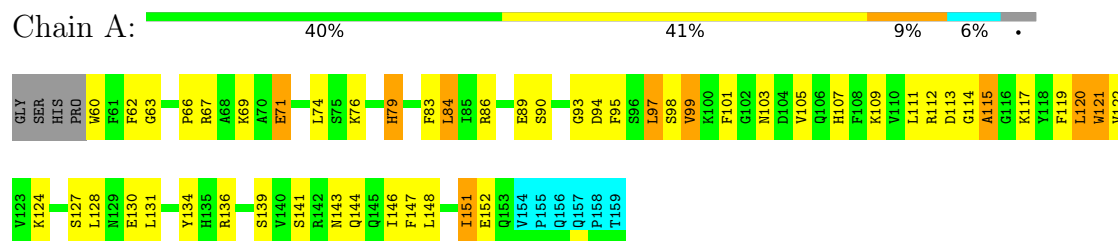
4.2.17 Score per residue for model 17

- Molecule 1: Growth factor receptor-bound protein 2



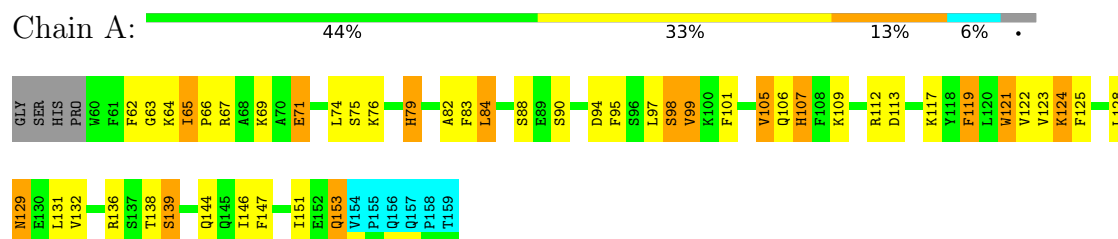
4.2.18 Score per residue for model 18

- Molecule 1: Growth factor receptor-bound protein 2



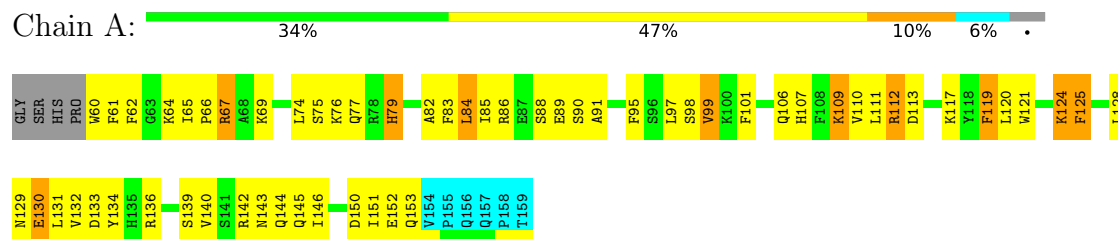
4.2.19 Score per residue for model 19

- Molecule 1: Growth factor receptor-bound protein 2



4.2.20 Score per residue for model 20

- 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.

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	36±9
2	A	49	43	43	2±2
All	All	16520	16040	16020	720

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 22.

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:84:LEU:O	1:A:84:LEU:HD23	0.83	1.72	19	15
1:A:62:PHE:CD1	1:A:84:LEU:HD11	0.83	2.09	16	8
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:97:LEU:C	1:A:97:LEU:HD13	0.78	2.04	15	11
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:LEU:HD23	1:A:84:LEU:C	0.75	2.06	20	11
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	0.71	2.10	16	2
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:60:TRP:CZ2	1:A:132:VAL:CG2	0.70	2.74	15	1
1:A:106:GLN:C	1:A:107:HIS:CD2	0.69	2.70	2	3
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	3
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:111:LEU:HD21	2:A:174:DTF:HAT1	0.66	1.65	5	2
1:A:83:PHE:C	1:A:83:PHE:CD1	0.66	2.74	8	7
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:122:VAL:O	1:A:122:VAL:HG23	0.65	1.90	11	1
1:A:124:LYS:C	1:A:125:PHE:CD1	0.64	2.75	2	5
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:CD1	1:A:125:PHE:N	0.62	2.68	11	4
1:A:84:LEU:HD23	1:A:84:LEU:O	0.62	1.95	6	2
1:A:135:HIS:ND1	1:A:140:VAL:HG12	0.61	2.09	4	1
1:A:60:TRP:CE2	1:A:132:VAL:HG11	0.61	2.30	20	1
1:A:114:GLY:O	1:A:115:ALA:HB2	0.61	1.94	5	2
1:A:135:HIS:CD2	1:A:148:LEU:HD21	0.61	2.31	12	1
1:A:125:PHE:CE1	1:A:131:LEU:HD21	0.60	2.31	11	1
1:A:65:ILE:HD11	1:A:84:LEU:HD21	0.60	1.72	15	3
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:CE2	0.60	2.31	10	7
1:A:99:VAL:HG11	1:A:101:PHE:CZ	0.60	2.32	2	18

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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:134:TYR:C	1:A:134:TYR:CD1	0.60	2.79	12	7
1:A:61:PHE:CE1	1:A:62:PHE:O	0.59	2.56	16	6
1:A:65:ILE:HD11	1:A:86:ARG:HB3	0.59	1.75	3	2
1:A:83:PHE:CE2	1:A:132:VAL:HG13	0.59	2.33	4	3
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:97:LEU:C	1:A:97:LEU:CD1	0.59	2.75	15	12
1:A:101:PHE:CE1	1:A:146:ILE:HD13	0.59	2.33	12	1
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	2
1:A:121:TRP:C	1:A:122:VAL:HG23	0.57	2.24	8	1
1:A:120:LEU:N	1:A:120:LEU:CD1	0.57	2.68	18	1
1:A:120:LEU:HD23	1:A:121:TRP:NE1	0.57	2.15	9	1
1:A:120:LEU:CD1	1:A:131:LEU:CD2	0.57	2.82	15	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:129:ASN:C	1:A:129:ASN:ND2	0.56	2.64	10	4
1:A:121:TRP:O	1:A:122:VAL:C	0.55	2.49	11	2
1:A:120:LEU:HD22	1:A:120:LEU:C	0.55	2.26	18	1
1:A:119:PHE:C	1:A:120:LEU:HD12	0.55	2.27	12	2
1:A:126:ASN:CG	1:A:127:SER:N	0.55	2.65	7	2
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:CD2	1:A:107:HIS:N	0.54	2.75	8	6
1:A:111:LEU:HD11	2:A:174:DTF:CAS	0.54	2.31	3	1
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:79:HIS:N	1:A:79:HIS:CD2	0.54	2.76	16	4
1:A:71:GLU:OE2	1:A:107:HIS:CE1	0.54	2.61	6	1
1:A:65:ILE:CD1	1:A:70:ALA:HB2	0.53	2.34	9	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:HIS:HB3	1:A:148:LEU:HD11	0.53	1.80	17	4
1:A:124:LYS:C	1:A:125:PHE:CG	0.53	2.87	2	6
1:A:71:GLU:N	1:A:71:GLU:OE1	0.52	2.43	6	1
1:A:119:PHE:CD1	1:A:119:PHE:N	0.52	2.78	10	4
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:66:PRO:O	1:A:67:ARG:C	0.51	2.53	12	12
1:A:71:GLU:OE1	1:A:71:GLU:N	0.51	2.43	18	2
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:112:ARG:HG2	1:A:118:TYR:CD1	0.51	2.41	2	3
1:A:83:PHE:CZ	1:A:132:VAL:CG1	0.51	2.94	6	5
1:A:107:HIS:C	1:A:108:PHE:CD1	0.51	2.89	8	3
1:A:111:LEU:C	1:A:119:PHE:CE1	0.51	2.89	20	3
1:A:111:LEU:HB3	1:A:119:PHE:CE1	0.51	2.40	4	3
1:A:111:LEU:HD21	2:A:174:DTF:CBQ	0.51	2.36	2	1
1:A:129:ASN:ND2	1:A:130:GLU:N	0.51	2.59	13	1
1:A:135:HIS:ND1	1:A:140:VAL:CG1	0.50	2.74	4	1
1:A:112:ARG:HA	1:A:119:PHE:CE1	0.50	2.41	20	1
1:A:79:HIS:CD2	1:A:79:HIS:N	0.50	2.78	9	15
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:135:HIS:NE2	1:A:140:VAL:HG22	0.50	2.22	12	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:111:LEU:HD11	2:A:174:DTF:CBQ	0.50	2.37	3	1
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:120:LEU:CB	1:A:121:TRP:CD1	0.49	2.95	14	1
1:A:123:VAL:HG22	1:A:124:LYS:N	0.49	2.23	2	2
1:A:146:ILE:HG22	1:A:147:PHE:N	0.49	2.22	12	10
1:A:133:ASP:O	1:A:136:ARG:N	0.49	2.45	20	5
1:A:118:TYR:HB2	1:A:131:LEU:HD13	0.49	1.83	8	1
1:A:71:GLU:O	1:A:75:SER:CB	0.49	2.60	19	1
1:A:116:GLY:O	1:A:118:TYR:CE1	0.49	2.65	1	1
1:A:120:LEU:O	1:A:122:VAL:N	0.49	2.45	18	2
1:A:129:ASN:OD1	1:A:129:ASN:C	0.49	2.56	3	1
1:A:114:GLY:O	1:A:115:ALA:CB	0.48	2.59	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:PHE:CE1	1:A:128:LEU:CD1	0.48	2.96	15	2
1:A:111:LEU:HD11	2:A:174:DTF:HAS1	0.48	1.85	2	1
1:A:84:LEU:C	1:A:84:LEU:CD2	0.48	2.85	18	5
1:A:135:HIS:CE1	1:A:140:VAL:HG23	0.48	2.42	10	1
1:A:152:GLU:O	1:A:152:GLU:CG	0.48	2.60	17	1
1:A:83:PHE:CD2	1:A:148:LEU:HD23	0.48	2.43	6	2
1:A:135:HIS:CB	1:A:148:LEU:CD1	0.48	2.92	14	1
1:A:120:LEU:HD12	1:A:131:LEU:CD2	0.48	2.39	18	1
1:A:121:TRP:CD1	1:A:122:VAL:HG13	0.48	2.42	5	1
1:A:95:PHE:CD1	1:A:128:LEU:CD1	0.48	2.97	20	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:140:VAL:HG22	1:A:140:VAL:O	0.48	2.08	14	1
1:A:74:LEU:HD23	1:A:151:ILE:HG13	0.48	1.84	18	1
1:A:135:HIS:CG	1:A:140:VAL:CG1	0.48	2.96	4	1
1:A:119:PHE:CB	1:A:123:VAL:O	0.48	2.62	1	1
1:A:74:LEU:HD11	1:A:98:SER:OG	0.48	2.09	8	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:140:VAL:HG22	1:A:146:ILE:O	0.47	2.09	11	1
1:A:135:HIS:CD2	1:A:140:VAL:HG12	0.47	2.43	15	1
1:A:71:GLU:OE1	1:A:71:GLU:CA	0.47	2.62	18	1
1:A:111:LEU:CD1	2:A:174:DTF:CAT	0.47	2.91	20	1
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:66:PRO:O	1:A:69:LYS:N	0.47	2.47	15	3
1:A:97:LEU:HD23	1:A:108:PHE:CD2	0.47	2.45	10	1
1:A:152:GLU:O	1:A:153:GLN:C	0.47	2.56	3	2
1:A:120:LEU:C	1:A:120:LEU:CD2	0.47	2.88	18	1
1:A:62:PHE:CD1	1:A:84:LEU:HD12	0.47	2.44	5	1
1:A:112:ARG:HG2	1:A:118:TYR:CD2	0.47	2.45	11	1
1:A:125:PHE:CD1	1:A:130:GLU:HB3	0.47	2.45	12	1
1:A:128:LEU:O	1:A:131:LEU:N	0.47	2.48	9	3
1:A:71:GLU:OE2	1:A:105:VAL:CG1	0.47	2.63	6	1
1:A:65:ILE:HD13	1:A:70:ALA:HB2	0.47	1.86	12	1
1:A:93:GLY:O	1:A:112:ARG:CZ	0.47	2.63	18	1
1:A:133:ASP:O	1:A:134:TYR:C	0.47	2.58	2	4
1:A:121:TRP:CH2	2:A:174:DTF:HB1	0.47	2.44	14	1
1:A:125:PHE:CD2	1:A:130:GLU:HB3	0.46	2.45	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:60:TRP:HA	1:A:83:PHE:CE1	0.46	2.45	13	1
1:A:125:PHE:CG	1:A:130:GLU:HB3	0.46	2.46	14	2
1:A:63:GLY:O	1:A:64:LYS:C	0.46	2.57	16	1
1:A:83:PHE:CD2	1:A:148:LEU:CD2	0.46	2.99	8	1
1:A:120:LEU:HB3	1:A:121:TRP:CD1	0.46	2.44	14	1
1:A:60:TRP:CB	1:A:83:PHE:CE1	0.46	2.98	2	1
1:A:112:ARG:C	1:A:119:PHE:CZ	0.46	2.94	16	2
1:A:135:HIS:CE1	1:A:140:VAL:HG12	0.46	2.46	4	1
1:A:60:TRP:CH2	1:A:85:ILE:HD12	0.46	2.46	20	1
1:A:125:PHE:CG	1:A:131:LEU:HD11	0.46	2.45	11	2
1:A:128:LEU:O	1:A:129:ASN:C	0.46	2.59	9	3
1:A:121:TRP:C	1:A:123:VAL:N	0.46	2.74	12	1
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:84:LEU:O	1:A:84:LEU:CD2	0.45	2.60	7	3
1:A:123:VAL:CG2	1:A:125:PHE:CE2	0.45	3.00	7	1
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:71:GLU:OE2	1:A:107:HIS:NE2	0.45	2.50	18	2
1:A:125:PHE:CE1	1:A:130:GLU:OE1	0.45	2.70	13	1
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:110:VAL:O	1:A:112:ARG:NH2	0.45	2.50	2	1
1:A:97:LEU:O	1:A:107:HIS:CB	0.45	2.64	12	2
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:121:TRP:CD1	1:A:121:TRP:C	0.45	2.94	5	1
1:A:86:ARG:NH2	2:A:174:DTF:OAF	0.44	2.50	2	3
1:A:97:LEU:HD11	1:A:99:VAL:HG23	0.44	1.90	2	3
1:A:60:TRP:CB	1:A:83:PHE:CE2	0.44	3.00	7	2
1:A:99:VAL:CG2	1:A:148:LEU:HD22	0.44	2.42	18	1
1:A:110:VAL:C	1:A:111:LEU:HD22	0.44	2.37	20	1
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	3
1:A:94:ASP:OD1	1:A:94:ASP:C	0.44	2.61	16	1
1:A:67:ARG:NH2	2:A:174:DTF:OAH	0.44	2.50	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:ASN:O	1:A:132:VAL:HG22	0.44	2.12	5	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
1:A:138:THR:O	1:A:139:SER:C	0.44	2.61	2	9
1:A:107:HIS:CD2	2:A:174:DTF:CBO	0.44	3.00	1	1
1:A:60:TRP:N	1:A:151:ILE:HG22	0.44	2.27	18	2
1:A:71:GLU:CD	1:A:105:VAL:CG1	0.44	2.91	4	1
1:A:107:HIS:CD2	2:A:174:DTF:HBC2	0.44	2.48	15	2
1:A:71:GLU:HG2	1:A:105:VAL:CG1	0.44	2.43	19	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:152:GLU:CG	1:A:152:GLU:O	0.43	2.65	1	1
1:A:60:TRP:HB2	1:A:83:PHE:CE1	0.43	2.48	2	2
1:A:129:ASN:CG	1:A:130:GLU:N	0.43	2.76	6	1
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:120:LEU:HB3	1:A:121:TRP:NE1	0.43	2.28	14	1
1:A:60:TRP:CG	1:A:83:PHE:CZ	0.43	3.06	8	1
1:A:85:ILE:HG22	1:A:95:PHE:CD1	0.43	2.49	11	1
1:A:123:VAL:HG22	1:A:125:PHE:CZ	0.43	2.49	15	1
1:A:62:PHE:CZ	1:A:73:MET:HG3	0.43	2.49	16	1
1:A:73:MET:N	1:A:73:MET:HE2	0.43	2.29	10	1
1:A:65:ILE:O	1:A:65:ILE:CD1	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:125:PHE:CE1	1:A:131:LEU:CD2	0.42	3.02	11	1
1:A:135:HIS:CG	1:A:140:VAL:HG12	0.42	2.49	15	1
1:A:99:VAL:HG21	1:A:148:LEU:CD1	0.42	2.44	4	1
1:A:123:VAL:CG2	1:A:125:PHE:CZ	0.42	3.02	15	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:125:PHE:CD2	1:A:131:LEU:HG	0.42	2.49	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:SER:O	1:A:131:LEU:HD12	0.42	2.15	11	1
1:A:60:TRP:HB3	1:A:151:ILE:HG22	0.42	1.90	16	1
1:A:130:GLU:O	1:A:134:TYR:CB	0.42	2.68	20	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	6	3
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:121:TRP:CD1	1:A:121:TRP:H	0.42	2.33	7	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:120:LEU:O	1:A:121:TRP:C	0.41	2.63	18	1
1:A:111:LEU:N	1:A:111:LEU:HD22	0.41	2.30	1	1
1:A:121:TRP:CH2	2:A:174:DTF:HA1	0.41	2.51	14	2
1:A:111:LEU:CD2	2:A:174:DTF:CAS	0.41	2.98	12	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:99:VAL:HG21	1:A:148:LEU:CD2	0.41	2.45	18	2
1:A:101:PHE:CE1	1:A:146:ILE:HD12	0.41	2.50	20	1
1:A:111:LEU:HD22	1:A:111:LEU:N	0.41	2.30	20	1
1:A:112:ARG:N	1:A:119:PHE:CE1	0.41	2.88	20	1
1:A:85:ILE:CG2	1:A:95:PHE:CD1	0.41	3.03	11	1
1:A:134:TYR:O	1:A:138:THR:HG22	0.41	2.16	5	1
1:A:112:ARG:C	1:A:113:ASP:OD1	0.41	2.63	6	1
1:A:135:HIS:O	1:A:138:THR:O	0.41	2.39	14	1
1:A:71:GLU:CD	1:A:105:VAL:HB	0.41	2.40	18	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:119:PHE:N	1:A:119:PHE:CD1	0.41	2.89	2	2
1:A:106:GLN:C	1:A:107:HIS:CG	0.41	2.99	7	1
1:A:119:PHE:HB3	1:A:124:LYS:CB	0.40	2.46	7	1
1:A:97:LEU:HG	1:A:98:SER:N	0.40	2.31	10	1
1:A:79:HIS:CD2	1:A:79:HIS:H	0.40	2.33	14	1
1:A:63:GLY:O	1:A:64:LYS:O	0.40	2.39	16	1
1:A:118:TYR:CD1	1:A:118:TYR:N	0.40	2.89	1	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:83:PHE:CZ	1:A:132:VAL:HG13	0.40	2.51	2	1
1:A:60:TRP:N	1:A:153:GLN:OE1	0.40	2.55	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:PHE:CZ	1:A:128:LEU:CD1	0.40	3.02	16	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%)	4	32
All	All	1860/2080 (89%)	1561 (84%)	231 (12%)	68 (4%)	4	32

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	153	GLN	5
1	A	121	TRP	5
1	A	122	VAL	4
1	A	88	SER	2
1	A	77	GLN	1
1	A	79	HIS	1
1	A	116	GLY	1
1	A	67	ARG	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%)	58±3 (70±4%)	25±3 (30±4%)	1	17
All	All	1660/1840 (90%)	1168 (70%)	492 (30%)	1	17

All 60 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	99	VAL	20
1	A	109	LYS	19
1	A	69	LYS	18
1	A	124	LYS	16
1	A	112	ARG	15
1	A	86	ARG	14
1	A	107	HIS	14
1	A	64	LYS	13
1	A	141	SER	13
1	A	144	GLN	13
1	A	65	ILE	12
1	A	76	LYS	12
1	A	90	SER	12
1	A	150	ASP	12
1	A	89	GLU	11
1	A	129	ASN	11
1	A	143	ASN	11
1	A	153	GLN	11
1	A	131	LEU	11
1	A	151	ILE	11
1	A	119	PHE	10
1	A	136	ARG	10
1	A	88	SER	10
1	A	103	ASN	10
1	A	120	LEU	10
1	A	94	ASP	10
1	A	84	LEU	10
1	A	117	LYS	9
1	A	113	ASP	8
1	A	98	SER	8
1	A	127	SER	8
1	A	130	GLU	7
1	A	133	ASP	7
1	A	152	GLU	7
1	A	135	HIS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	142	ARG	6
1	A	67	ARG	5
1	A	75	SER	5
1	A	137	SER	5
1	A	96	SER	4
1	A	111	LEU	4
1	A	148	LEU	4
1	A	71	GLU	4
1	A	138	THR	4
1	A	145	GLN	4
1	A	121	TRP	3
1	A	125	PHE	3
1	A	104	ASP	3
1	A	126	ASN	3
1	A	78	ARG	2
1	A	80	ASP	2
1	A	100	LYS	2
1	A	83	PHE	2
1	A	122	VAL	2
1	A	97	LEU	2
1	A	118	TYR	1
1	A	134	TYR	1
1	A	139	SER	1
1	A	105	VAL	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 oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

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	-	53,53,53	1.50±0.00	11±0 (20±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	-	70,75,75	1.51±0.00	13±0 (18±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

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
2	A	174	DTF	CBO-CBS	3.42	1.56	1.52	8	20
2	A	174	DTF	CBV-CBM	3.41	1.60	1.53	5	20
2	A	174	DTF	PBW-CBF	3.36	1.74	1.79	17	20
2	A	174	DTF	CAZ-CBV	3.08	1.58	1.54	9	20
2	A	174	DTF	CBA-CBV	2.91	1.57	1.54	3	20
2	A	174	DTF	CBB-CBT	2.86	1.57	1.52	17	20
2	A	174	DTF	CBV-NBI	2.39	1.50	1.46	17	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	174	DTF	CBC-CBS	2.25	1.56	1.54	1	20
2	A	174	DTF	PBW-OAG	2.23	1.54	1.50	8	20
2	A	174	DTF	CA-C	2.16	1.58	1.52	4	20
2	A	174	DTF	PBW-OAF	2.08	1.59	1.55	9	20

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

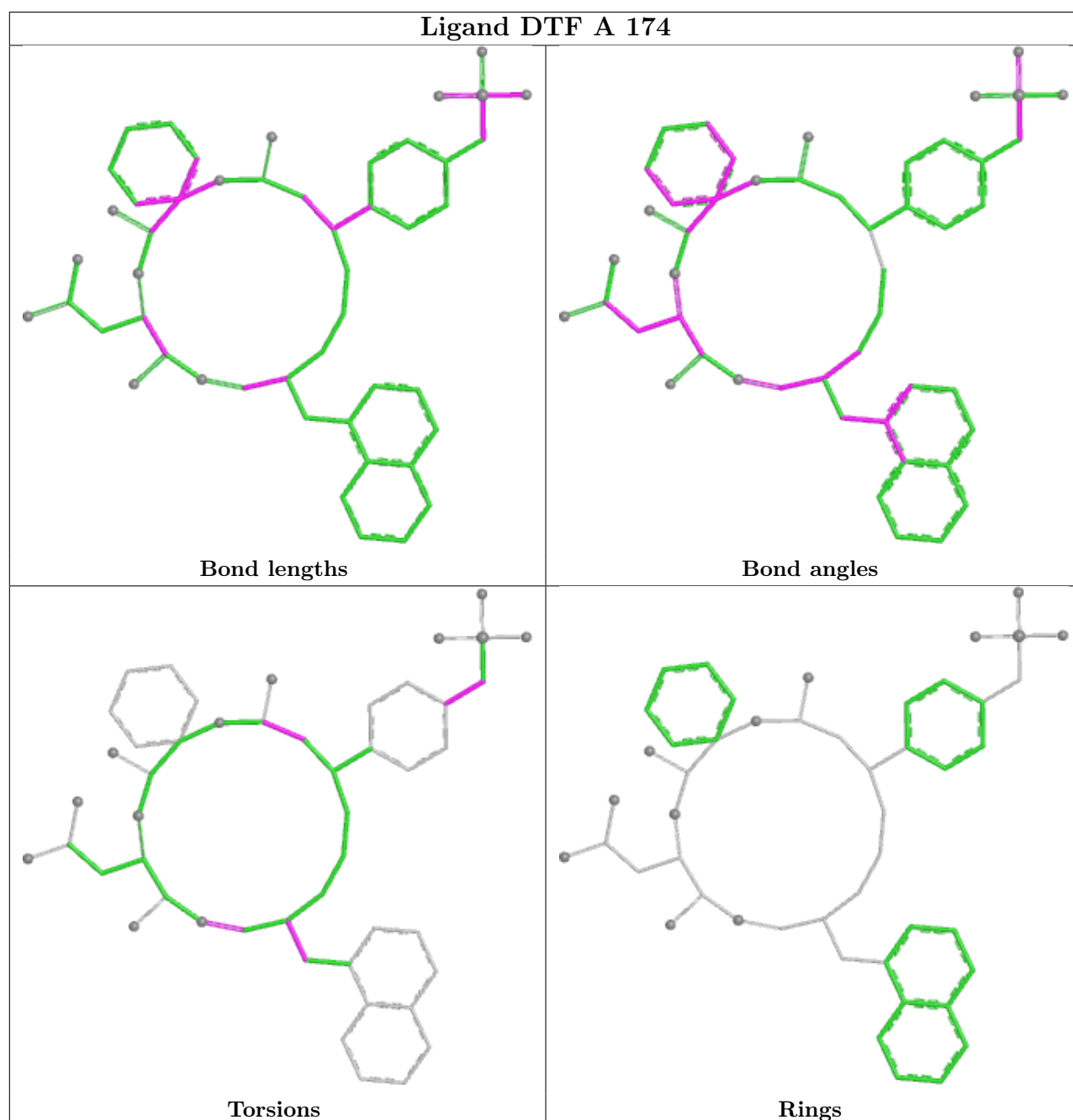
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	174	DTF	CBB-CBT-CAY	6.02	118.49	110.18	19	20
2	A	174	DTF	CAW-CAZ-CBV	3.53	117.56	112.39	15	20
2	A	174	DTF	CBM-CBV-NBI	3.47	116.13	110.05	19	20
2	A	174	DTF	CBA-CBV-NBI	3.22	103.44	109.57	17	20
2	A	174	DTF	CA-CB-CG	2.84	117.91	112.21	12	20
2	A	174	DTF	CB-CA-N	2.78	105.33	110.64	6	20
2	A	174	DTF	CAX-CBA-CBV	2.59	116.18	112.39	12	20
2	A	174	DTF	CB-CA-C	2.46	116.37	110.57	20	20
2	A	174	DTF	CBE-CBP-CBR	2.30	124.23	120.89	9	20
2	A	174	DTF	OAH-PBW-CBF	2.28	112.42	106.78	1	20
2	A	174	DTF	CBT-CBB-NBG	2.12	116.46	112.77	18	20
2	A	174	DTF	CBE-CBP-CAP	2.11	116.57	119.92	12	20
2	A	174	DTF	C-CA-N	2.06	116.69	111.11	11	20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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