



Full wwPDB NMR Structure Validation Report ⓘ

May 31, 2020 – 10:35 pm BST

PDB ID : 6HD2
Title : Active-site conformational dynamics of carbonic anhydrase II under native conditions: An NMR perspective
Authors : Singh, H.; Linser, R.
Deposited on : 2018-08-17

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 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
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

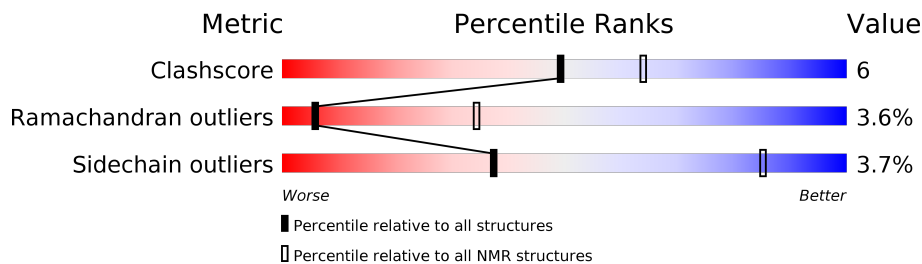
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 72%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	260	

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:32-A:196, A:203-A:260 (223)	0.89	1

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

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

The models can be grouped into 2 clusters and 5 single-model clusters were found.

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

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4112 atoms, of which 2037 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Carbonic anhydrase 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	260	4108	1329	2035	357	384	3	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	1	1	1

- Molecule 3 is water.

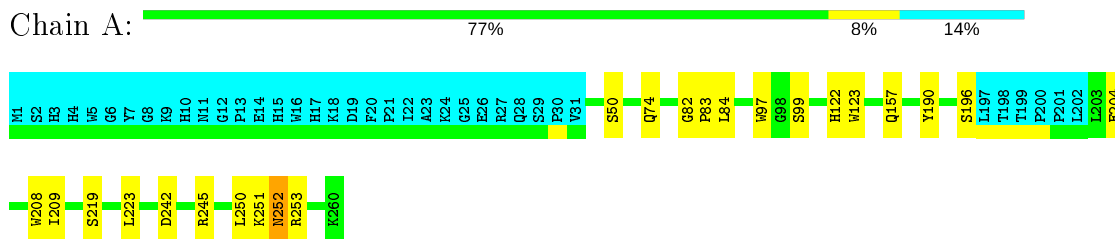
Mol	Chain	Residues	Atoms		
			Total	H	O
3	A	1	3	2	1

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: Carbonic anhydrase 2

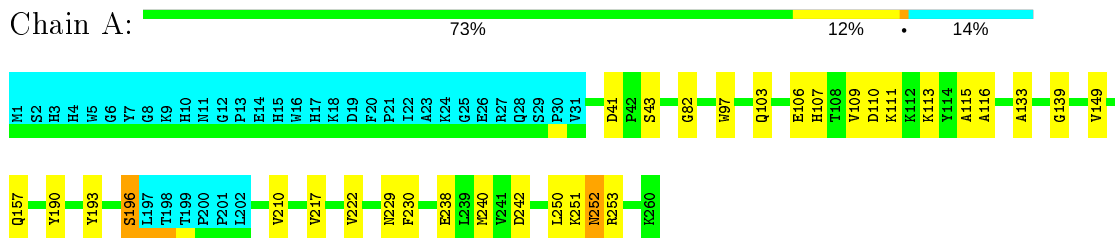


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

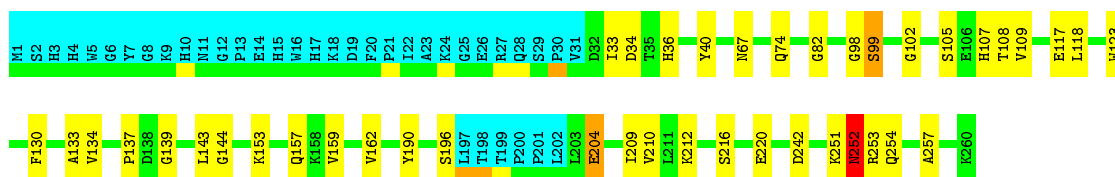
- Molecule 1: Carbonic anhydrase 2



4.2.2 Score per residue for model 2

- Molecule 1: Carbonic anhydrase 2

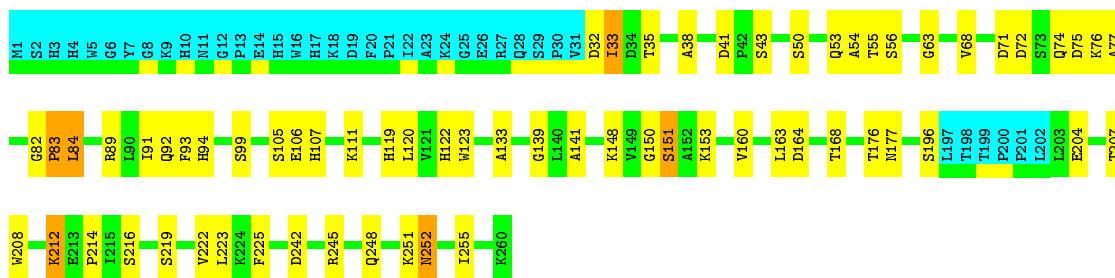




4.2.3 Score per residue for model 3

- Molecule 1: Carbonic anhydrase 2

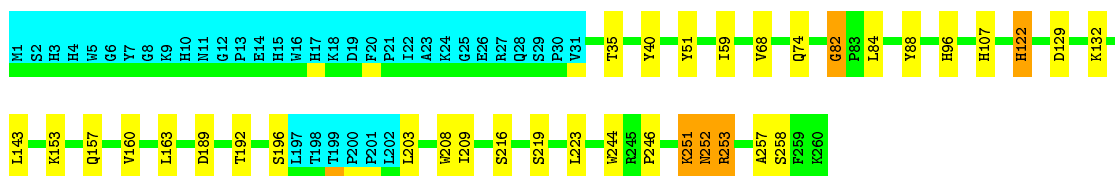
Chain A: 60% 23% 14%



4.2.4 Score per residue for model 4

- Molecule 1: Carbonic anhydrase 2

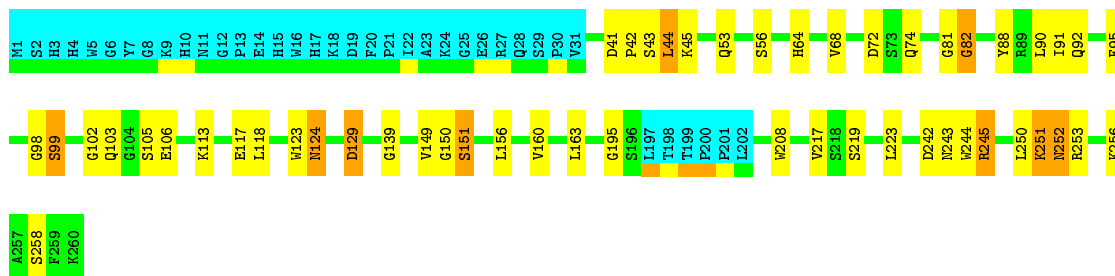
Chain A: 72% 12% 14%



4.2.5 Score per residue for model 5

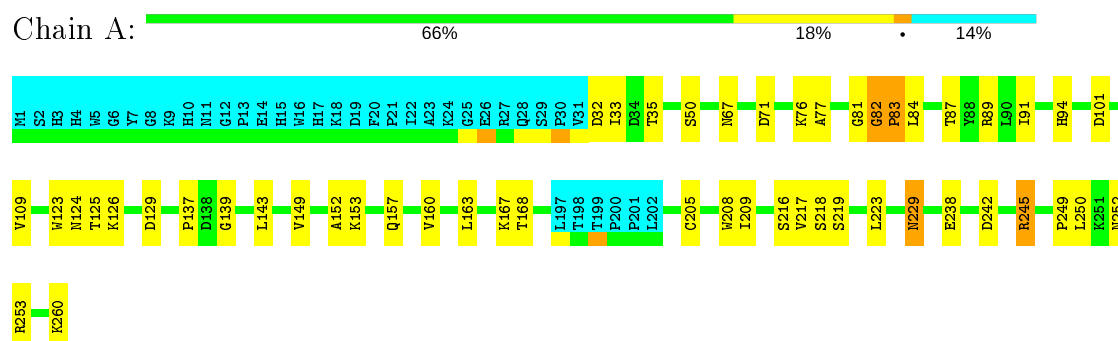
- Molecule 1: Carbonic anhydrase 2

Chain A: 66% 17% 14%



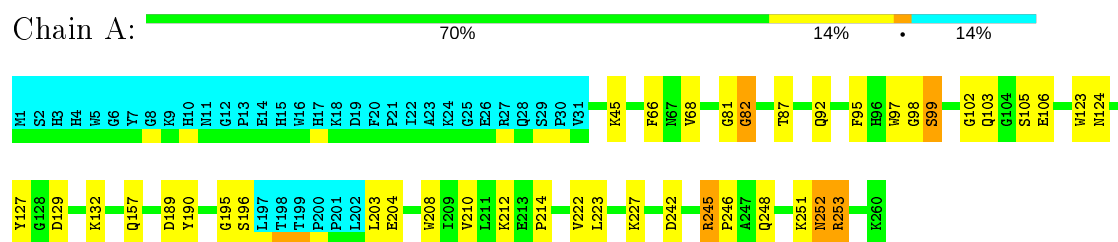
4.2.6 Score per residue for model 6

- Molecule 1: Carbonic anhydrase 2



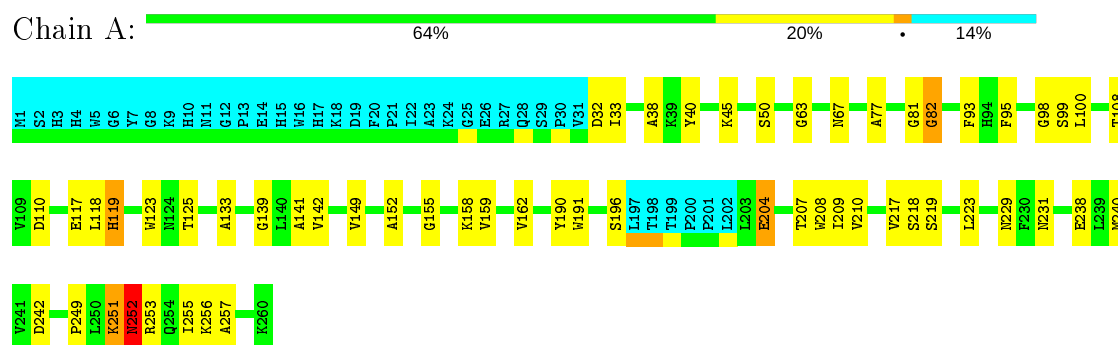
4.2.7 Score per residue for model 7

- Molecule 1: Carbonic anhydrase 2



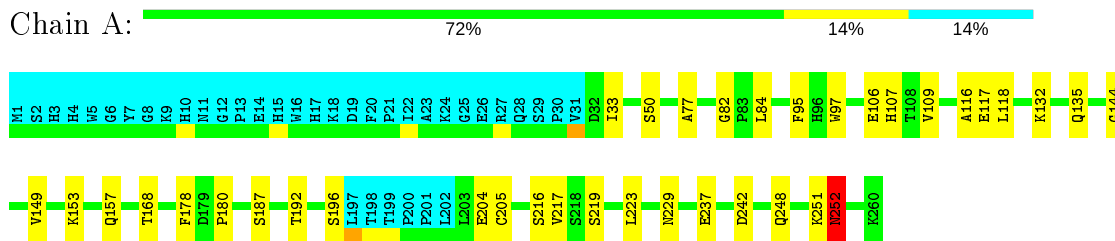
4.2.8 Score per residue for model 8

- Molecule 1: Carbonic anhydrase 2



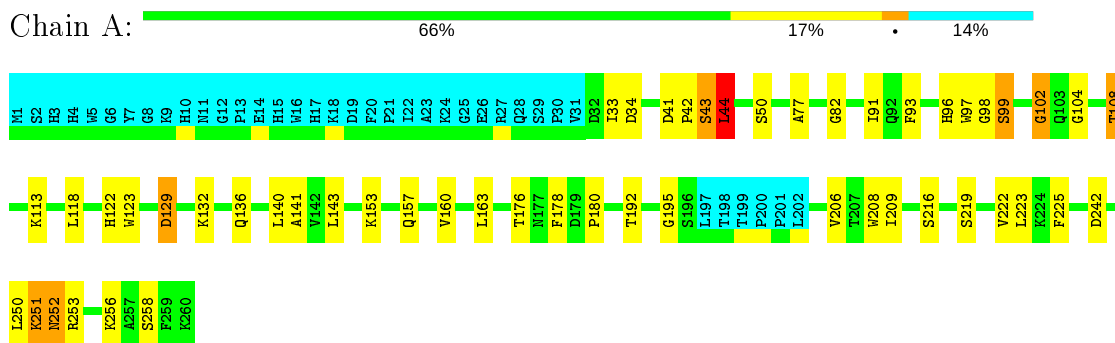
4.2.9 Score per residue for model 9

- Molecule 1: Carbonic anhydrase 2



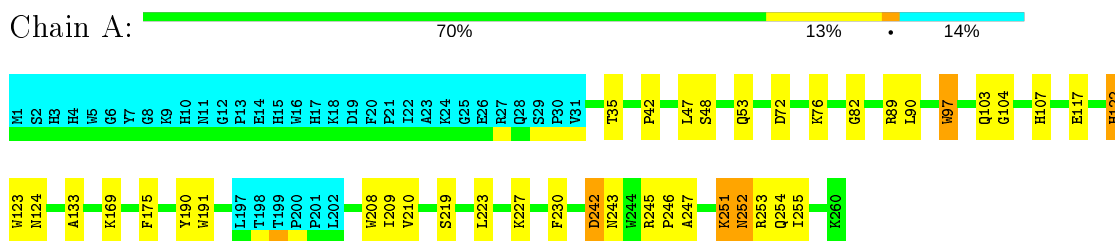
4.2.10 Score per residue for model 10

- Molecule 1: Carbonic anhydrase 2



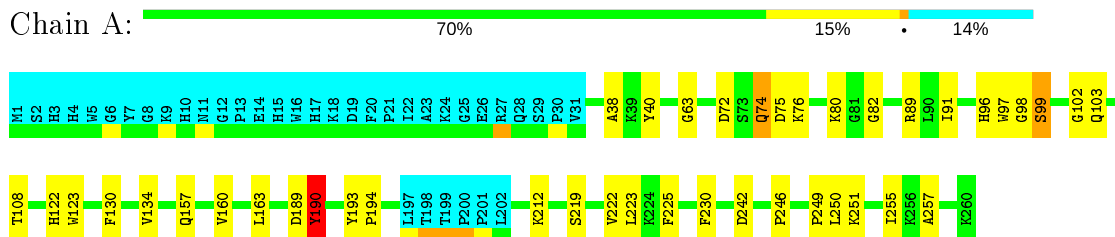
4.2.11 Score per residue for model 11

- Molecule 1: Carbonic anhydrase 2



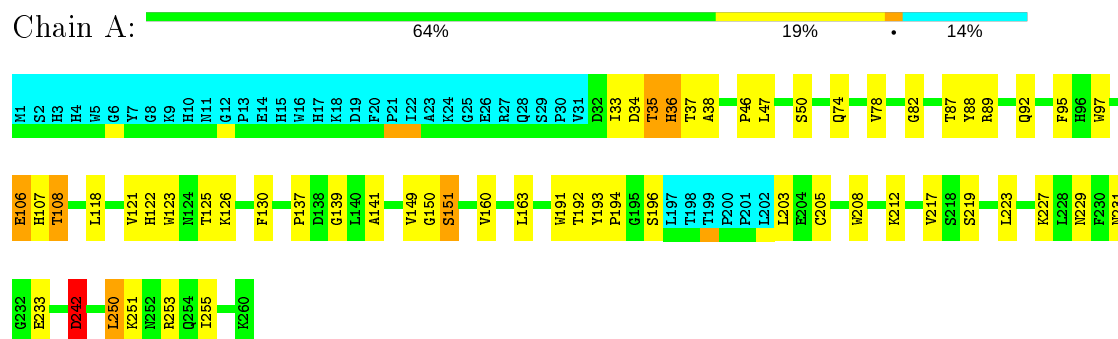
4.2.12 Score per residue for model 12

- Molecule 1: Carbonic anhydrase 2



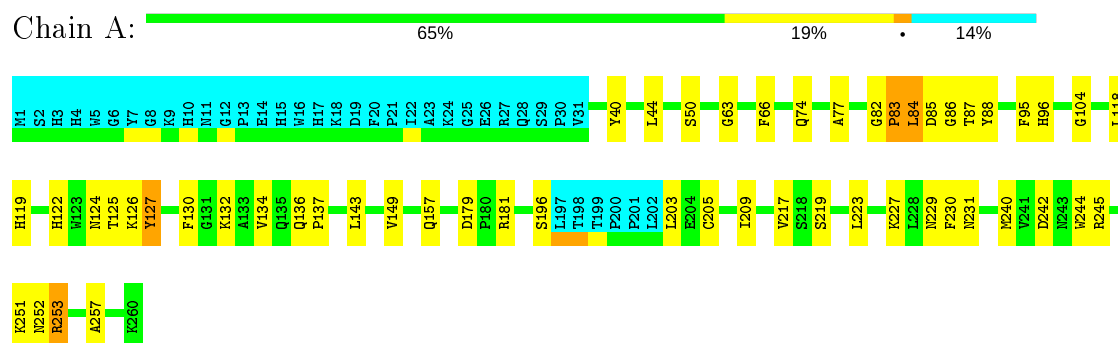
4.2.13 Score per residue for model 13

- Molecule 1: Carbonic anhydrase 2



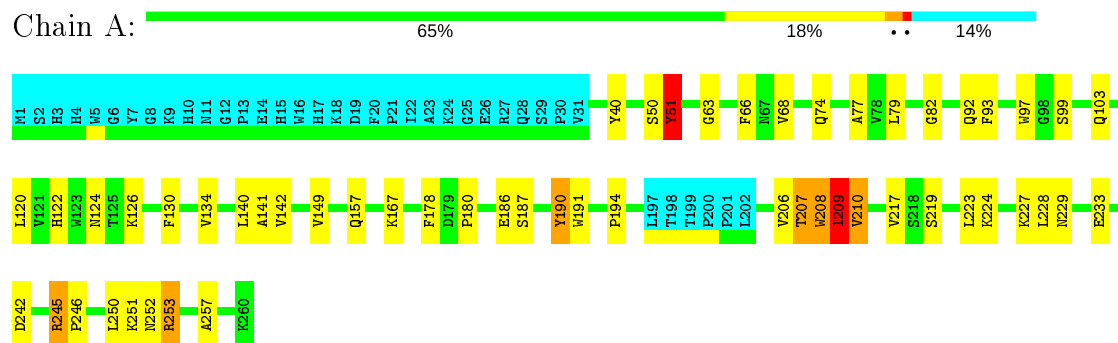
4.2.14 Score per residue for model 14

- Molecule 1: Carbonic anhydrase 2



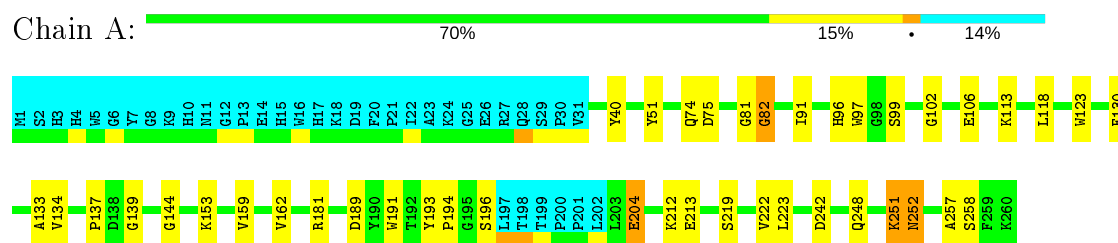
4.2.15 Score per residue for model 15

- Molecule 1: Carbonic anhydrase 2



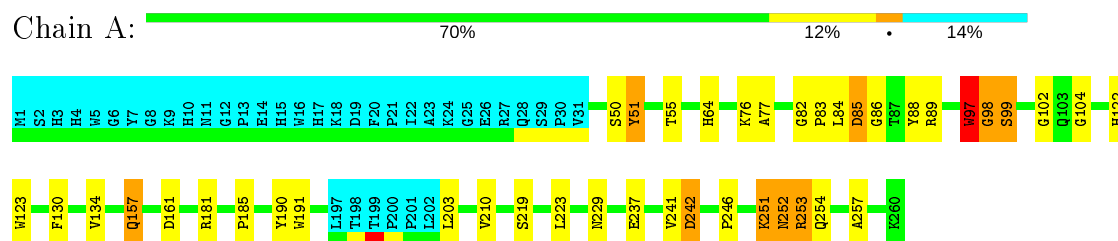
4.2.16 Score per residue for model 16

- Molecule 1: Carbonic anhydrase 2



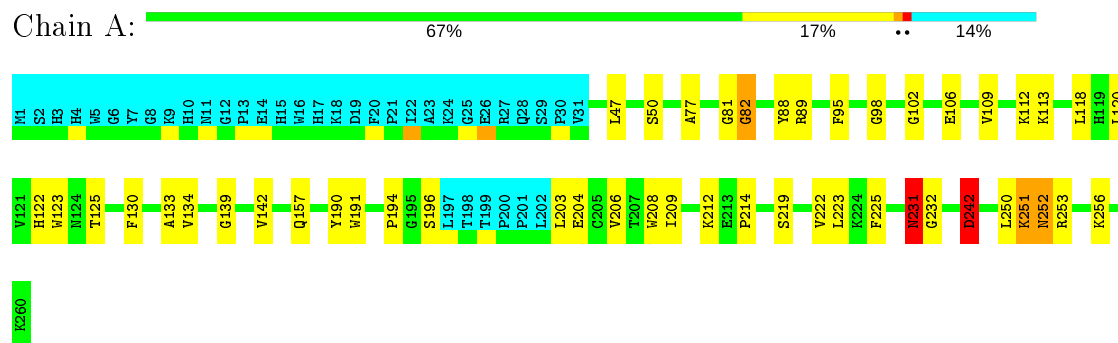
4.2.17 Score per residue for model 17

- Molecule 1: Carbonic anhydrase 2



4.2.18 Score per residue for model 18

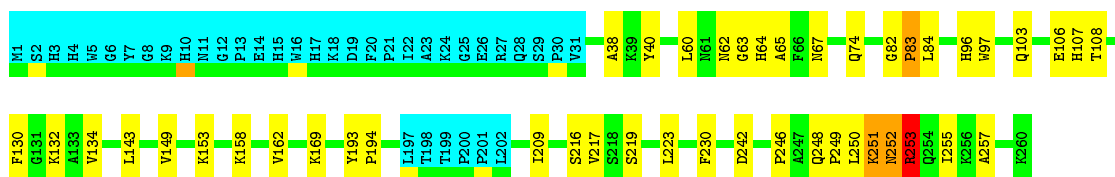
- Molecule 1: Carbonic anhydrase 2



4.2.19 Score per residue for model 19

- Molecule 1: Carbonic anhydrase 2





4.2.20 Score per residue for model 20

- Molecule 1: Carbonic anhydrase 2

Chain A: 65% 18% 14%



5 Refinement protocol and experimental data overview (i)

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

Of the 500 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CNS	refinement	
ARIA	structure calculation	2.3

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	2269
Number of shifts mapped to atoms	2268
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	1
Assignment completeness (well-defined parts)	72%

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

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	1770	1746	1742	21±6
All	All	35440	34960	34840	426

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:ILE:O	1:A:109:VAL:HA	0.67	1.90	6	3
1:A:87:THR:O	1:A:124:ASN:HA	0.66	1.90	7	1
1:A:40:TYR:HA	1:A:257:ALA:O	0.65	1.90	4	8
1:A:208:TRP:O	1:A:209:ILE:HG12	0.64	1.93	20	1
1:A:55:THR:HB	1:A:71:ASP:OD1	0.64	1.93	3	1
1:A:149:VAL:HA	1:A:217:VAL:O	0.64	1.91	8	9
1:A:195:GLY:HA3	1:A:208:TRP:CD1	0.63	2.29	5	2
1:A:88:TYR:HA	1:A:122:HIS:CD2	0.62	2.29	4	1
1:A:251:LYS:O	1:A:252:ASN:HB2	0.62	1.94	8	5
1:A:190:TYR:HA	1:A:210:VAL:O	0.61	1.96	7	6
1:A:50:SER:O	1:A:77:ALA:HA	0.61	1.96	9	10
1:A:160:VAL:O	1:A:163:LEU:HG	0.61	1.96	13	8
1:A:219:SER:O	1:A:223:LEU:HG	0.60	1.96	20	17
1:A:68:VAL:O	1:A:92:GLN:HA	0.60	1.96	3	4
1:A:222:VAL:HA	1:A:225:PHE:CD2	0.60	2.30	12	5
1:A:191:TRP:CE3	1:A:257:ALA:HB2	0.59	2.32	17	1
1:A:33:ILE:O	1:A:110:ASP:HA	0.59	1.96	8	1
1:A:66:PHE:CE1	1:A:228:LEU:HD13	0.59	2.32	15	1
1:A:43:SER:O	1:A:44:LEU:HG	0.59	1.98	10	1
1:A:251:LYS:O	1:A:252:ASN:HB3	0.59	1.97	18	3
1:A:133:ALA:O	1:A:139:GLY:HA3	0.58	1.98	18	7
1:A:91:ILE:HB	1:A:123:TRP:CD1	0.57	2.35	10	2
1:A:123:TRP:CD1	1:A:130:PHE:HB2	0.57	2.35	13	1
1:A:95:PHE:CZ	1:A:118:LEU:HD13	0.57	2.35	9	2
1:A:224:LYS:O	1:A:228:LEU:HG	0.57	1.99	15	1
1:A:32:ASP:HA	1:A:108:THR:OG1	0.56	2.00	8	1
1:A:195:GLY:O	1:A:206:VAL:HB	0.56	2.00	10	1
1:A:124:ASN:OD1	1:A:126:LYS:HG2	0.56	2.00	6	3
1:A:41:ASP:O	1:A:258:SER:HA	0.56	2.00	5	2
1:A:196:SER:HA	1:A:203:LEU:O	0.56	2.00	4	3
1:A:97:TRP:O	1:A:242:ASP:HA	0.56	2.01	13	1
1:A:123:TRP:CZ3	1:A:125:THR:HA	0.55	2.35	18	3
1:A:150:GLY:O	1:A:151:SER:HB2	0.55	2.01	5	3
1:A:95:PHE:CE2	1:A:118:LEU:HG	0.55	2.37	8	1
1:A:253:ARG:HD2	1:A:253:ARG:O	0.55	2.02	1	1
1:A:250:LEU:HA	1:A:253:ARG:O	0.55	2.01	18	4
1:A:142:VAL:O	1:A:209:ILE:HB	0.55	2.02	20	1
1:A:98:GLY:HA2	1:A:242:ASP:H	0.55	1.60	18	1
1:A:251:LYS:O	1:A:253:ARG:N	0.54	2.39	19	4
1:A:97:TRP:CB	1:A:104:GLY:HA2	0.54	2.32	17	1
1:A:223:LEU:O	1:A:227:LYS:HG2	0.54	2.02	7	3
1:A:203:LEU:HD13	1:A:205:CYS:SG	0.54	2.43	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:TRP:CD1	1:A:242:ASP:HA	0.54	2.38	11	1
1:A:98:GLY:HA3	1:A:103:GLN:O	0.53	2.02	5	1
1:A:91:ILE:HD12	1:A:123:TRP:CE3	0.53	2.38	12	2
1:A:253:ARG:NE	1:A:253:ARG:HA	0.53	2.19	19	1
1:A:124:ASN:ND2	1:A:133:ALA:HB2	0.53	2.19	11	1
1:A:132:LYS:O	1:A:136:GLN:HG2	0.52	2.04	20	1
1:A:249:PRO:O	1:A:253:ARG:HD3	0.52	2.04	8	1
1:A:250:LEU:HG	1:A:251:LYS:N	0.52	2.19	12	1
1:A:230:PHE:CE1	1:A:240:MET:HA	0.52	2.40	14	1
1:A:191:TRP:O	1:A:209:ILE:HA	0.52	2.05	11	1
1:A:97:TRP:CH2	1:A:222:VAL:HB	0.52	2.39	12	3
1:A:143:LEU:HA	1:A:209:ILE:O	0.52	2.05	2	5
1:A:95:PHE:CZ	1:A:118:LEU:HG	0.52	2.40	8	1
1:A:129:ASP:OD2	1:A:140:LEU:HG	0.51	2.05	10	1
1:A:97:TRP:CZ3	1:A:222:VAL:HB	0.51	2.40	10	2
1:A:159:VAL:O	1:A:162:VAL:HG12	0.51	2.05	2	3
1:A:87:THR:HB	1:A:125:THR:OG1	0.51	2.06	14	1
1:A:124:ASN:ND2	1:A:129:ASP:HA	0.51	2.20	5	1
1:A:130:PHE:O	1:A:134:VAL:HG23	0.51	2.05	12	8
1:A:193:TYR:CD1	1:A:251:LYS:HD2	0.51	2.40	12	1
1:A:178:PHE:O	1:A:180:PRO:HD3	0.51	2.05	9	3
1:A:204:GLU:O	1:A:204:GLU:HG3	0.51	2.05	7	1
1:A:98:GLY:O	1:A:99:SER:HB2	0.51	2.05	5	6
1:A:72:ASP:OD1	1:A:89:ARG:HD2	0.51	2.06	11	3
1:A:38:ALA:HA	1:A:255:ILE:O	0.50	2.06	19	4
1:A:190:TYR:CD2	1:A:212:LYS:HA	0.50	2.41	12	1
1:A:89:ARG:HG2	1:A:123:TRP:O	0.50	2.06	12	1
1:A:248:GLN:HB3	1:A:249:PRO:HD2	0.50	1.84	19	1
1:A:153:LYS:HG2	1:A:216:SER:O	0.50	2.06	10	3
1:A:34:ASP:C	1:A:36:HIS:H	0.50	2.10	13	1
1:A:137:PRO:HA	1:A:204:GLU:O	0.50	2.06	2	2
1:A:33:ILE:HB	1:A:108:THR:O	0.49	2.07	13	2
1:A:229:ASN:ND2	1:A:237:GLU:HG3	0.49	2.23	17	2
1:A:85:ASP:CG	1:A:86:GLY:H	0.49	2.11	20	2
1:A:84:LEU:HG	1:A:84:LEU:O	0.49	2.07	3	2
1:A:167:LYS:HE2	1:A:229:ASN:OD1	0.49	2.08	15	1
1:A:189:ASP:HB3	1:A:258:SER:O	0.49	2.06	4	2
1:A:54:ALA:HB2	1:A:77:ALA:HB2	0.49	1.85	3	1
1:A:119:HIS:CD2	1:A:142:VAL:HB	0.48	2.43	8	1
1:A:105:SER:O	1:A:106:GLU:HB3	0.48	2.09	5	3
1:A:191:TRP:HA	1:A:256:LYS:O	0.48	2.08	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:245:ARG:HD3	1:A:246:PRO:O	0.48	2.08	15	1
1:A:89:ARG:O	1:A:122:HIS:HA	0.48	2.09	18	4
1:A:252:ASN:O	1:A:253:ARG:HB2	0.48	2.09	7	1
1:A:229:ASN:HA	1:A:238:GLU:O	0.48	2.09	8	4
1:A:229:ASN:HB3	1:A:231:ASN:OD1	0.48	2.09	8	3
1:A:97:TRP:NE1	1:A:99:SER:HA	0.48	2.24	15	1
1:A:157:GLN:HE21	1:A:157:GLN:HA	0.47	1.69	17	1
1:A:192:THR:HA	1:A:208:TRP:O	0.47	2.09	4	2
1:A:212:LYS:O	1:A:214:PRO:HD3	0.47	2.09	3	3
1:A:231:ASN:OD1	1:A:237:GLU:HA	0.47	2.09	20	1
1:A:140:LEU:C	1:A:206:VAL:HG12	0.47	2.29	15	1
1:A:42:PRO:O	1:A:44:LEU:HD23	0.47	2.09	10	1
1:A:163:LEU:HD12	1:A:164:ASP:N	0.47	2.23	3	1
1:A:55:THR:OG1	1:A:76:LYS:HE2	0.47	2.09	17	1
1:A:66:PHE:CZ	1:A:95:PHE:HB2	0.47	2.43	14	1
1:A:156:LEU:O	1:A:160:VAL:HG23	0.47	2.10	20	2
1:A:88:TYR:HB3	1:A:122:HIS:HB3	0.47	1.86	14	2
1:A:152:ALA:HB2	1:A:218:SER:CB	0.47	2.39	8	1
1:A:193:TYR:CD2	1:A:194:PRO:HD2	0.47	2.45	13	2
1:A:63:GLY:HA2	1:A:240:MET:SD	0.47	2.49	8	1
1:A:118:LEU:O	1:A:144:GLY:HA2	0.47	2.09	9	3
1:A:95:PHE:CE2	1:A:118:LEU:HD13	0.47	2.44	18	3
1:A:245:ARG:HD2	1:A:245:ARG:O	0.47	2.10	5	1
1:A:47:LEU:HG	1:A:190:TYR:CE2	0.47	2.44	18	1
1:A:98:GLY:O	1:A:241:VAL:HA	0.47	2.10	17	1
1:A:231:ASN:CG	1:A:232:GLY:H	0.47	2.13	18	1
1:A:253:ARG:N	1:A:253:ARG:HD3	0.47	2.25	4	1
1:A:129:ASP:OD2	1:A:132:LYS:HG2	0.46	2.09	20	2
1:A:93:PHE:CB	1:A:120:LEU:HA	0.46	2.40	20	3
1:A:104:GLY:O	1:A:244:TRP:HB2	0.46	2.11	14	1
1:A:106:GLU:HA	1:A:244:TRP:NE1	0.46	2.26	5	1
1:A:190:TYR:CD1	1:A:209:ILE:HG23	0.46	2.45	18	1
1:A:79:LEU:HB2	1:A:122:HIS:CE1	0.46	2.46	15	1
1:A:98:GLY:CA	1:A:104:GLY:HA3	0.46	2.40	10	1
1:A:67:ASN:HA	1:A:93:PHE:O	0.46	2.10	8	1
1:A:137:PRO:HA	1:A:205:CYS:SG	0.46	2.51	13	1
1:A:245:ARG:CD	1:A:245:ARG:H	0.46	2.23	7	1
1:A:44:LEU:HG	1:A:45:LYS:H	0.46	1.70	5	1
1:A:189:ASP:O	1:A:212:LYS:HB2	0.46	2.10	12	1
1:A:220:GLU:CD	1:A:220:GLU:H	0.46	2.14	2	1
1:A:103:GLN:O	1:A:115:ALA:HA	0.46	2.11	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:HIS:C	1:A:38:ALA:H	0.46	2.15	13	1
1:A:107:HIS:HE2	1:A:117:GLU:CD	0.46	2.14	11	1
1:A:191:TRP:HB3	1:A:257:ALA:HA	0.46	1.88	15	1
1:A:106:GLU:CD	1:A:107:HIS:H	0.45	2.14	13	1
1:A:191:TRP:HB3	1:A:255:ILE:CG2	0.45	2.41	13	1
1:A:191:TRP:CZ2	1:A:212:LYS:HG3	0.45	2.45	16	1
1:A:88:TYR:O	1:A:124:ASN:HA	0.45	2.11	5	1
1:A:194:PRO:HA	1:A:206:VAL:O	0.45	2.11	18	1
1:A:252:ASN:HD22	1:A:252:ASN:C	0.45	2.13	9	1
1:A:122:HIS:O	1:A:141:ALA:HA	0.45	2.11	13	1
1:A:250:LEU:HD12	1:A:251:LYS:N	0.45	2.27	13	1
1:A:120:LEU:O	1:A:142:VAL:HA	0.45	2.11	18	1
1:A:53:GLN:HB2	1:A:76:LYS:O	0.45	2.11	11	2
1:A:50:SER:HB2	1:A:78:VAL:O	0.45	2.11	13	1
1:A:251:LYS:O	1:A:252:ASN:CB	0.45	2.64	11	9
1:A:94:HIS:NE2	1:A:119:HIS:HB2	0.45	2.27	3	1
1:A:62:ASN:HB3	1:A:67:ASN:OD1	0.45	2.11	19	1
1:A:56:SER:O	1:A:176:THR:HA	0.45	2.11	3	1
1:A:92:GLN:O	1:A:121:VAL:HB	0.45	2.12	13	1
1:A:71:ASP:O	1:A:76:LYS:HD2	0.45	2.12	6	1
1:A:206:VAL:O	1:A:206:VAL:HG23	0.45	2.11	15	1
1:A:127:TYR:CE1	1:A:132:LYS:HB3	0.45	2.46	14	1
1:A:194:PRO:HA	1:A:207:THR:OG1	0.45	2.12	15	1
1:A:230:PHE:CE2	1:A:240:MET:HA	0.45	2.47	1	1
1:A:122:HIS:HB2	1:A:141:ALA:O	0.45	2.12	15	2
1:A:44:LEU:HG	1:A:45:LYS:N	0.45	2.27	5	1
1:A:87:THR:O	1:A:125:THR:HG22	0.44	2.12	6	2
1:A:153:LYS:HB2	1:A:216:SER:O	0.44	2.12	6	3
1:A:93:PHE:CD2	1:A:118:LEU:HD11	0.44	2.47	10	1
1:A:74:GLN:NE2	1:A:76:LYS:HE2	0.44	2.27	12	1
1:A:191:TRP:CZ3	1:A:212:LYS:HA	0.44	2.47	13	1
1:A:208:TRP:O	1:A:209:ILE:HG23	0.44	2.13	15	1
1:A:209:ILE:N	1:A:209:ILE:HD13	0.44	2.27	15	1
1:A:97:TRP:HE1	1:A:222:VAL:HB	0.44	1.73	1	1
1:A:193:TYR:CB	1:A:255:ILE:HG12	0.44	2.43	13	1
1:A:167:LYS:O	1:A:229:ASN:HB2	0.44	2.12	6	1
1:A:97:TRP:HA	1:A:242:ASP:O	0.44	2.13	17	1
1:A:192:THR:OG1	1:A:256:LYS:HB2	0.44	2.12	10	1
1:A:72:ASP:OD1	1:A:90:LEU:HB3	0.44	2.13	5	1
1:A:141:ALA:HA	1:A:207:THR:O	0.44	2.13	8	2
1:A:231:ASN:N	1:A:231:ASN:HD22	0.44	2.09	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:223:LEU:O	1:A:227:LYS:HG3	0.44	2.12	11	1
1:A:193:TYR:CD1	1:A:194:PRO:HD2	0.44	2.48	12	1
1:A:107:HIS:NE2	1:A:117:GLU:OE1	0.44	2.50	9	1
1:A:250:LEU:C	1:A:252:ASN:H	0.44	2.15	1	1
1:A:204:GLU:H	1:A:204:GLU:CD	0.43	2.16	8	1
1:A:63:GLY:O	1:A:230:PHE:HB2	0.43	2.12	12	1
1:A:66:PHE:CZ	1:A:95:PHE:HB3	0.43	2.48	7	1
1:A:88:TYR:HA	1:A:122:HIS:NE2	0.43	2.27	4	1
1:A:41:ASP:OD2	1:A:43:SER:HB3	0.43	2.12	3	1
1:A:51:TYR:CE1	1:A:181:ARG:HA	0.43	2.48	17	1
1:A:35:THR:O	1:A:37:THR:N	0.43	2.51	13	1
1:A:90:LEU:HA	1:A:122:HIS:HB3	0.43	1.89	11	1
1:A:84:LEU:O	1:A:84:LEU:HG	0.43	2.14	20	1
1:A:179:ASP:CG	1:A:181:ARG:HE	0.43	2.17	20	1
1:A:142:VAL:O	1:A:209:ILE:HG21	0.43	2.13	15	1
1:A:81:GLY:O	1:A:82:GLY:O	0.43	2.36	5	6
1:A:190:TYR:HB2	1:A:209:ILE:HG23	0.43	1.90	8	1
1:A:91:ILE:HB	1:A:123:TRP:CE3	0.43	2.49	16	1
1:A:88:TYR:HB3	1:A:122:HIS:CB	0.43	2.44	14	1
1:A:67:ASN:ND2	1:A:94:HIS:HB3	0.43	2.29	6	1
1:A:109:VAL:O	1:A:112:LYS:HB3	0.43	2.14	18	1
1:A:88:TYR:HA	1:A:123:TRP:O	0.43	2.14	18	1
1:A:98:GLY:HA2	1:A:242:ASP:N	0.43	2.29	18	1
1:A:106:GLU:HG3	1:A:245:ARG:O	0.43	2.14	3	1
1:A:121:VAL:HA	1:A:141:ALA:HB1	0.42	1.91	13	1
1:A:132:LYS:O	1:A:135:GLN:HG2	0.42	2.13	9	1
1:A:82:GLY:O	1:A:84:LEU:HG	0.42	2.13	4	1
1:A:89:ARG:HD2	1:A:123:TRP:CZ2	0.42	2.49	6	2
1:A:132:LYS:O	1:A:136:GLN:HG3	0.42	2.14	10	1
1:A:169:LYS:HD2	1:A:230:PHE:O	0.42	2.15	11	1
1:A:106:GLU:HG2	1:A:107:HIS:N	0.42	2.29	3	1
1:A:196:SER:HA	1:A:204:GLU:HA	0.42	1.91	3	1
1:A:245:ARG:HD2	1:A:245:ARG:H	0.42	1.74	6	1
1:A:45:LYS:HB3	1:A:82:GLY:HA3	0.42	1.90	7	1
1:A:59:ILE:HG13	1:A:68:VAL:HG22	0.42	1.92	4	1
1:A:33:ILE:HB	1:A:109:VAL:HG22	0.42	1.91	2	1
1:A:155:GLY:O	1:A:158:LYS:HE2	0.42	2.14	8	1
1:A:88:TYR:CE1	1:A:139:GLY:HA3	0.42	2.50	13	1
1:A:140:LEU:HB2	1:A:206:VAL:HG21	0.42	1.91	20	1
1:A:193:TYR:CG	1:A:194:PRO:HD2	0.42	2.50	19	1
1:A:97:TRP:CE3	1:A:116:ALA:HB1	0.42	2.49	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:250:LEU:O	1:A:251:LYS:HD3	0.42	2.14	12	1
1:A:127:TYR:CG	1:A:132:LYS:HG3	0.42	2.50	7	1
1:A:148:LYS:O	1:A:216:SER:HA	0.42	2.14	3	1
1:A:102:GLY:O	1:A:113:LYS:HB2	0.42	2.14	10	1
1:A:89:ARG:HD3	1:A:125:THR:CB	0.42	2.45	13	1
1:A:208:TRP:CD1	1:A:210:VAL:HG22	0.42	2.49	8	1
1:A:51:TYR:CE1	1:A:181:ARG:HG2	0.42	2.49	16	1
1:A:250:LEU:HG	1:A:251:LYS:H	0.42	1.74	12	1
1:A:99:SER:HB3	1:A:103:GLN:NE2	0.42	2.30	7	1
1:A:136:GLN:O	1:A:205:CYS:HB3	0.41	2.14	14	1
1:A:158:LYS:O	1:A:162:VAL:HG23	0.41	2.15	19	1
1:A:62:ASN:O	1:A:64:HIS:N	0.41	2.53	19	1
1:A:193:TYR:O	1:A:207:THR:HB	0.41	2.14	20	1
1:A:193:TYR:OH	1:A:253:ARG:HA	0.41	2.15	1	1
1:A:137:PRO:HA	1:A:205:CYS:HA	0.41	1.92	14	1
1:A:42:PRO:C	1:A:44:LEU:H	0.41	2.19	5	1
1:A:65:ALA:CB	1:A:95:PHE:H	0.41	2.28	20	1
1:A:169:LYS:HD3	1:A:230:PHE:O	0.41	2.15	19	1
1:A:153:LYS:HG3	1:A:216:SER:O	0.41	2.14	9	1
1:A:51:TYR:CD1	1:A:180:PRO:HB2	0.41	2.50	15	1
1:A:97:TRP:CZ2	1:A:222:VAL:HB	0.41	2.51	7	1
1:A:52:ASP:HA	1:A:181:ARG:NH2	0.41	2.31	20	1
1:A:106:GLU:OE1	1:A:113:LYS:HD3	0.41	2.16	16	1
1:A:85:ASP:CG	1:A:86:GLY:N	0.41	2.74	17	1
1:A:64:HIS:CE1	1:A:243:ASN:HB3	0.41	2.50	5	1
1:A:109:VAL:O	1:A:111:LYS:N	0.41	2.54	1	1
1:A:179:ASP:OD1	1:A:181:ARG:HB3	0.41	2.16	14	1
1:A:143:LEU:HD12	1:A:209:ILE:O	0.41	2.15	14	1
1:A:137:PRO:O	1:A:205:CYS:HA	0.41	2.16	6	1
1:A:34:ASP:OD2	1:A:36:HIS:HB2	0.41	2.16	2	1
1:A:105:SER:HA	1:A:117:GLU:HB2	0.41	1.92	2	1
1:A:212:LYS:HD2	1:A:212:LYS:O	0.41	2.15	3	1
1:A:191:TRP:HB3	1:A:256:LYS:O	0.41	2.16	8	1
1:A:203:LEU:HB3	1:A:205:CYS:SG	0.41	2.56	20	1
1:A:191:TRP:CD1	1:A:210:VAL:HG21	0.41	2.50	15	1
1:A:252:ASN:O	1:A:253:ARG:HG2	0.40	2.15	19	1
1:A:46:PRO:O	1:A:47:LEU:HG	0.40	2.16	13	1
1:A:193:TYR:HB2	1:A:255:ILE:HA	0.40	1.93	20	1
1:A:123:TRP:HB2	1:A:129:ASP:CB	0.40	2.47	10	1
1:A:250:LEU:HD12	1:A:251:LYS:H	0.40	1.77	13	1
1:A:98:GLY:O	1:A:100:LEU:N	0.40	2.54	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:GLN:O	1:A:76:LYS:HB3	0.40	2.17	11	1
1:A:33:ILE:HB	1:A:248:GLN:CG	0.40	2.46	3	1
1:A:97:TRP:CD1	1:A:116:ALA:HB2	0.40	2.52	1	1
1:A:152:ALA:HA	1:A:218:SER:HB2	0.40	1.93	6	1
1:A:47:LEU:HD23	1:A:48:SER:N	0.40	2.31	11	1
1:A:105:SER:O	1:A:106:GLU:CB	0.40	2.68	3	1

5.2 Torsion angles [\(i\)](#)

5.2.1 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	222/260 (85%)	192±4 (87±2%)	22±4 (10±2%)	8±2 (4±1%)	6	34
All	All	4440/5200 (85%)	3844 (87%)	437 (10%)	159 (4%)	6	34

All 40 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	82	GLY	20
1	A	242	ASP	19
1	A	252	ASN	16
1	A	251	LYS	12
1	A	102	GLY	9
1	A	99	SER	9
1	A	253	ARG	8
1	A	246	PRO	6
1	A	84	LEU	6
1	A	83	PRO	6
1	A	129	ASP	4
1	A	63	GLY	4
1	A	75	ASP	3
1	A	44	LEU	3
1	A	151	SER	3
1	A	43	SER	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	97	TRP	2
1	A	139	GLY	2
1	A	209	ILE	2
1	A	64	HIS	2
1	A	190	TYR	2
1	A	98	GLY	1
1	A	100	LEU	1
1	A	187	SER	1
1	A	85	ASP	1
1	A	196	SER	1
1	A	231	ASN	1
1	A	110	ASP	1
1	A	113	LYS	1
1	A	101	ASP	1
1	A	123	TRP	1
1	A	42	PRO	1
1	A	36	HIS	1
1	A	65	ALA	1
1	A	249	PRO	1
1	A	35	THR	1
1	A	185	PRO	1
1	A	192	THR	1
1	A	91	ILE	1
1	A	104	GLY	1

5.2.2 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	193/225 (86%)	186±2 (96±1%)	7±2 (4±1%)	37 85
All	All	3860/4500 (86%)	3718 (96%)	142 (4%)	37 85

All 65 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	157	GLN	13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	74	GLN	11
1	A	96	HIS	7
1	A	106	GLU	5
1	A	108	THR	5
1	A	245	ARG	4
1	A	103	GLN	4
1	A	250	LEU	4
1	A	204	GLU	4
1	A	35	THR	4
1	A	252	ASN	4
1	A	208	TRP	4
1	A	254	GLN	3
1	A	242	ASP	3
1	A	168	THR	3
1	A	119	HIS	3
1	A	123	TRP	3
1	A	51	TYR	3
1	A	253	ARG	3
1	A	97	TRP	2
1	A	212	LYS	2
1	A	113	LYS	2
1	A	233	GLU	2
1	A	117	GLU	2
1	A	190	TYR	2
1	A	56	SER	1
1	A	127	TYR	1
1	A	176	THR	1
1	A	210	VAL	1
1	A	122	HIS	1
1	A	43	SER	1
1	A	243	ASN	1
1	A	80	LYS	1
1	A	45	LYS	1
1	A	187	SER	1
1	A	111	LYS	1
1	A	229	ASN	1
1	A	60	LEU	1
1	A	189	ASP	1
1	A	53	GLN	1
1	A	231	ASN	1
1	A	161	ASP	1
1	A	105	SER	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	124	ASN	1
1	A	107	HIS	1
1	A	227	LYS	1
1	A	251	LYS	1
1	A	175	PHE	1
1	A	44	LEU	1
1	A	33	ILE	1
1	A	41	ASP	1
1	A	203	LEU	1
1	A	34	ASP	1
1	A	260	LYS	1
1	A	67	ASN	1
1	A	256	LYS	1
1	A	213	GLU	1
1	A	132	LYS	1
1	A	244	TRP	1
1	A	209	ILE	1
1	A	186	GLU	1
1	A	126	LYS	1
1	A	153	LYS	1
1	A	177	ASN	1
1	A	84	LEU	1

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.5 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

5.6 Other polymers [i](#)

There are no such molecules in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 72% for the well-defined parts and 69% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

6.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	2269
Number of shifts mapped to atoms	2268
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	1
Number of shift outliers (ShiftChecker)	2

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atoms found in structure. The only occurrence is reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	94	HIS	HE3	7.629	0.02	1

6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	253	-0.01 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	229	0.28 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	249	0.07 ± 0.09	None needed (< 0.5 ppm)
^{15}N	237	1.05 ± 0.23	Should be applied

6.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 72%, i.e. 1976 atoms were assigned a chemical shift out of a possible 2757. 37 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	1069/1091 (98%)	419/434 (97%)	439/446 (98%)	211/211 (100%)
Sidechain	899/1398 (64%)	434/821 (53%)	442/519 (85%)	23/58 (40%)
Aromatic	8/268 (3%)	8/141 (6%)	0/111 (0%)	0/16 (0%)
Overall	1976/2757 (72%)	861/1396 (62%)	881/1076 (82%)	234/285 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 69%, i.e. 2224 atoms were assigned a chemical shift out of a possible 3234. 38 out of 43 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	1210/1266 (96%)	471/503 (94%)	502/520 (97%)	237/243 (98%)
Sidechain	1005/1619 (62%)	485/956 (51%)	494/597 (83%)	26/66 (39%)
Aromatic	9/349 (3%)	9/182 (5%)	0/139 (0%)	0/28 (0%)
Overall	2224/3234 (69%)	965/1641 (59%)	996/1256 (79%)	263/337 (78%)

6.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	123	TRP	HE3	12.23	9.33 – 5.33	12.3
1	A	244	TRP	HE3	10.49	9.33 – 5.33	7.9

6.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

