



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 03:27 AM BST

PDB ID : 2MM3  
Title : Solution NMR structure of the ternary complex of human ileal bile acid-binding protein with glycocholate and glycochenodeoxycholate  
Authors : Horvath, G.; Egyed, O.; Bencsura, A.; Simon, A.; Tochtrop, G.P.; DeKoster, G.T.; Covey, D.F.; Cistola, D.P.; Toke, O.  
Deposited on : 2014-03-07

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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

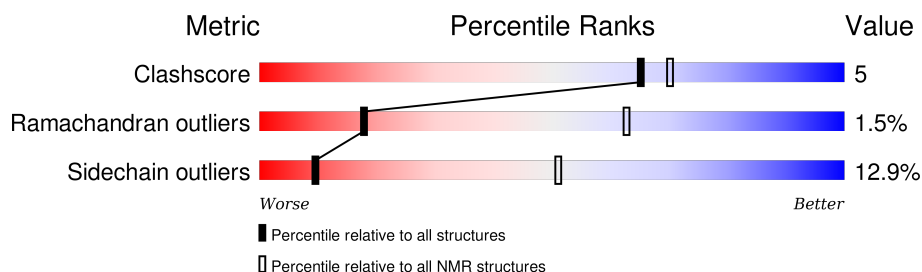
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 90%.

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  $\geq 3$ , 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	127	<div>82% 16% •</div>

## 2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:1-A:53, A:57-A:127 (124)	0.35	4

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

Cluster number	Models
1	4, 7, 8, 9
2	1, 5, 6
3	2, 3, 10

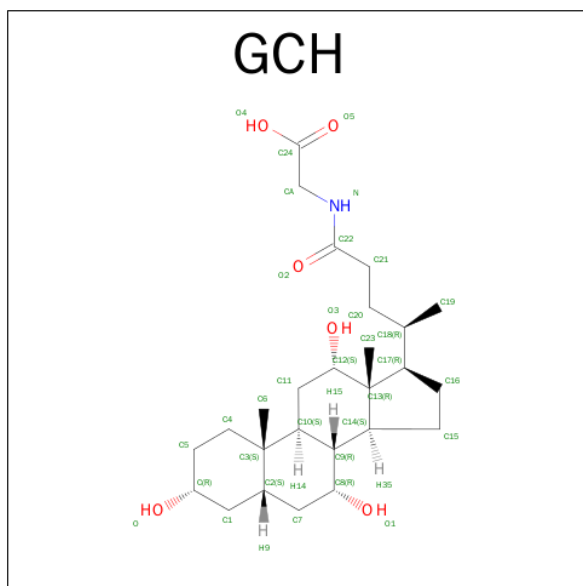
### 3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2133 atoms, of which 1067 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Gastrotropin.

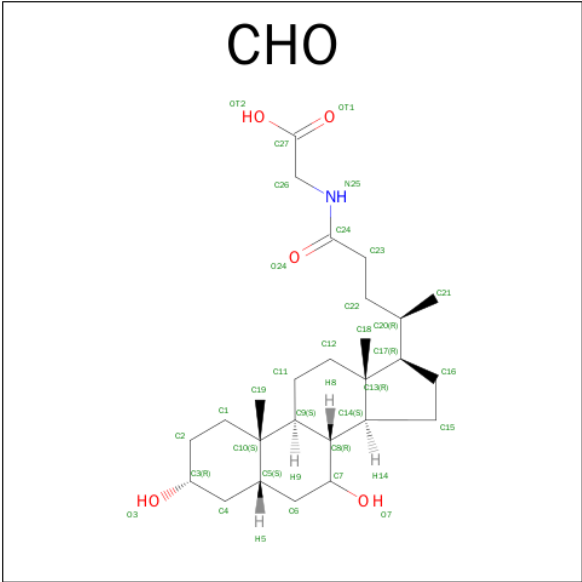
Mol	Chain	Residues	Atoms						Trace
1	A	127	Total	C	H	N	O	S	0
			1984	630	983	168	198	5	

- Molecule 2 is GLYCOCHOLIC ACID (three-letter code: GCH) (formula:  $C_{26}H_{43}NO_6$ ).



Mol	Chain	Residues	Atoms				
2	A	1	Total	C	H	N	O
			75	26	42	1	6

- Molecule 3 is GLYCOCHENODEOXYCHOLIC ACID (three-letter code: CHO) (formula:  $C_{26}H_{43}NO_5$ ).



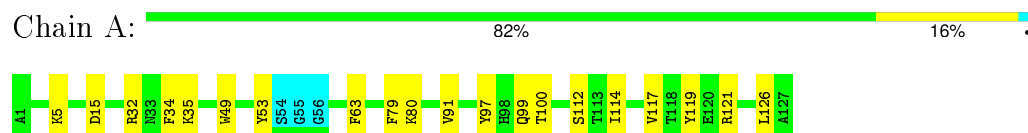
Mol	Chain	Residues	Atoms				
3	A	1	Total	C	H	N	O
			74	26	42	1	5

## 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: Gastrotropin

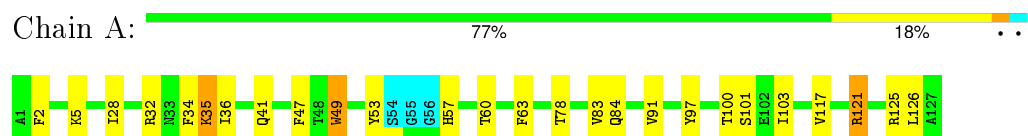


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

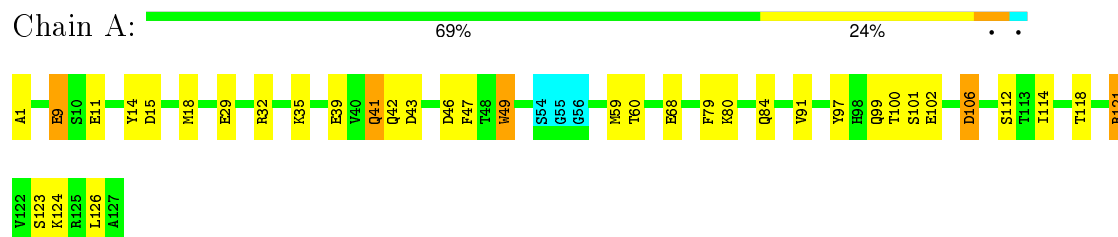
#### 4.2.1 Score per residue for model 1

- Molecule 1: Gastrotropin



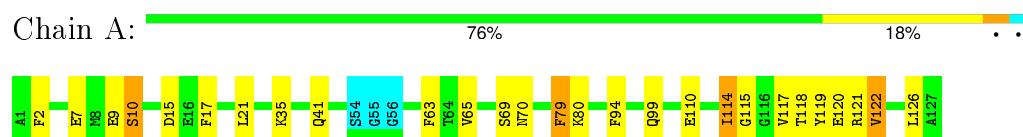
#### 4.2.2 Score per residue for model 2

- Molecule 1: Gastrotropin



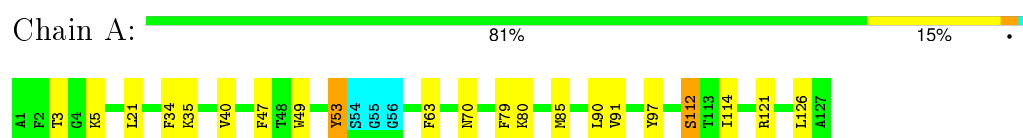
### 4.2.3 Score per residue for model 3

- Molecule 1: Gastrotropin



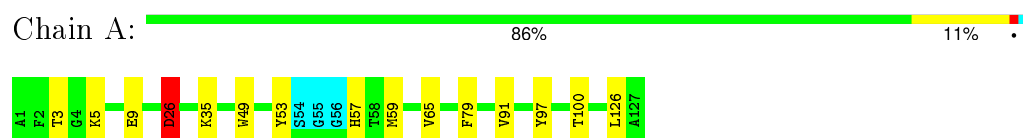
### 4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Gastrotropin



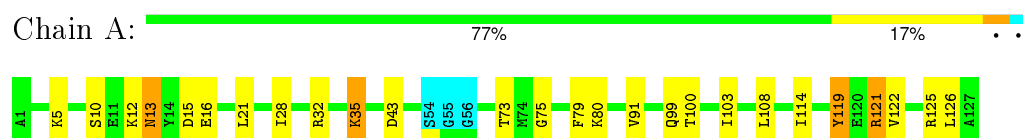
### 4.2.5 Score per residue for model 5

- Molecule 1: Gastrotropin



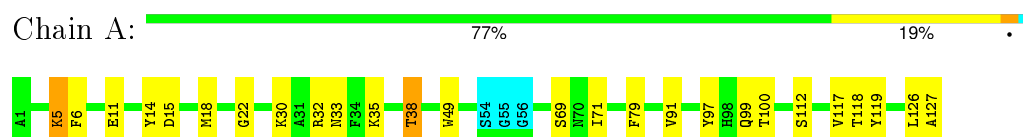
### 4.2.6 Score per residue for model 6

- Molecule 1: Gastrotropin



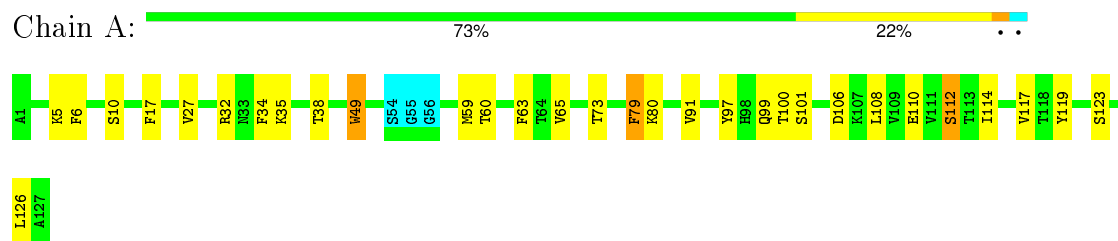
### 4.2.7 Score per residue for model 7

- Molecule 1: Gastrotropin



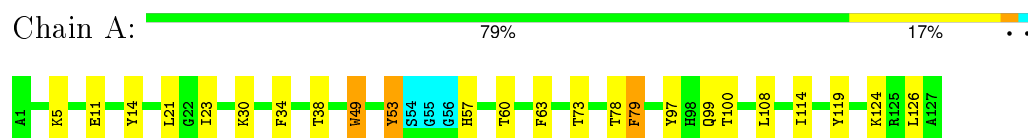
### 4.2.8 Score per residue for model 8

- Molecule 1: Gastrotropin



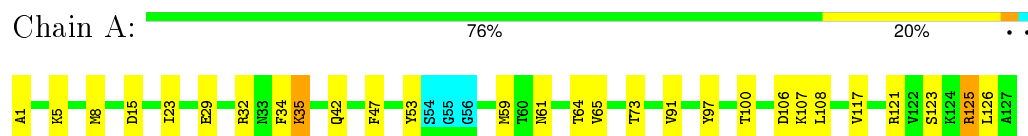
### 4.2.9 Score per residue for model 9

- Molecule 1: Gastrotropin



### 4.2.10 Score per residue for model 10

- Molecule 1: Gastrotropin





## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 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
ARIA	structure solution	2.1
ARIA	refinement	2.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	2mm3_cs.str
Number of chemical shift lists	1
Total number of shifts	1564
Number of shifts mapped to atoms	1564
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

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: GCH, CHO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.08±0.05	1±1/1004 (0.1±0.1%)	1.43±0.04	7±4/1346 (0.5±0.3%)
All	All	1.08	6/10040 (0.1%)	1.43	73/13460 (0.5%)

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
1	A	97	TYR	CG-CD2	5.67	1.46	1.39	5	1
1	A	16	GLU	CB-CG	5.62	1.62	1.52	6	1
1	A	69	SER	CA-CB	5.44	1.61	1.52	7	1
1	A	9	GLU	CD-OE1	-5.42	1.19	1.25	5	1
1	A	10	SER	CA-CB	5.37	1.61	1.52	3	1
1	A	123	SER	CA-CB	5.07	1.60	1.52	8	1

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
1	A	125	ARG	CG-CD-NE	-5.99	99.22	111.80	6	2
1	A	60	THR	O-C-N	-5.98	113.13	122.70	1	1
1	A	121	ARG	CG-CD-NE	5.96	124.31	111.80	2	1
1	A	14	TYR	CB-CG-CD2	-5.95	117.43	121.00	9	1
1	A	32	ARG	NE-CZ-NH1	5.95	123.27	120.30	8	5
1	A	15	ASP	CB-CG-OD2	-5.94	112.95	118.30	6	3
1	A	46	ASP	CB-CG-OD1	-5.94	112.95	118.30	2	1
1	A	121	ARG	CD-NE-CZ	5.94	131.91	123.60	2	2
1	A	7	GLU	O-C-N	-5.94	113.20	122.70	3	1
1	A	121	ARG	NE-CZ-NH1	5.94	123.27	120.30	1	3
1	A	32	ARG	CG-CD-NE	-5.93	99.34	111.80	1	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	106	ASP	CB-CG-OD1	5.91	123.61	118.30	2	2
1	A	53	TYR	CB-CG-CD2	-5.91	117.46	121.00	10	4
1	A	97	TYR	CB-CG-CD1	-5.90	117.46	121.00	1	4
1	A	119	TYR	CB-CG-CD1	5.90	124.54	121.00	6	1
1	A	9	GLU	O-C-N	-5.90	113.26	122.70	3	1
1	A	2	PHE	CB-CG-CD2	-5.89	116.68	120.80	3	1
1	A	125	ARG	NE-CZ-NH1	5.88	123.24	120.30	1	1
1	A	47	PHE	CB-CG-CD1	-5.87	116.69	120.80	2	1
1	A	15	ASP	CB-CG-OD1	5.86	123.57	118.30	2	1
1	A	12	LYS	O-C-N	-5.84	113.35	122.70	6	1
1	A	106	ASP	CB-CG-OD2	5.83	123.55	118.30	8	1
1	A	6	PHE	CB-CG-CD1	-5.80	116.74	120.80	7	1
1	A	26	ASP	CB-CG-OD2	5.77	123.49	118.30	5	1
1	A	120	GLU	O-C-N	-5.75	113.50	122.70	3	1
1	A	119	TYR	CA-CB-CG	5.73	124.29	113.40	6	1
1	A	63	PHE	CB-CG-CD1	-5.73	116.79	120.80	9	2
1	A	97	TYR	CB-CG-CD2	5.72	124.43	121.00	5	1
1	A	119	TYR	CG-CD1-CE1	-5.72	116.72	121.30	9	1
1	A	122	VAL	CB-CA-C	-5.72	100.53	111.40	3	1
1	A	119	TYR	CB-CG-CD2	-5.71	117.58	121.00	6	1
1	A	43	ASP	CB-CG-OD2	5.68	123.41	118.30	2	2
1	A	29	GLU	OE1-CD-OE2	-5.58	116.60	123.30	2	1
1	A	14	TYR	CZ-CE2-CD2	5.57	124.81	119.80	9	1
1	A	49	TRP	CA-CB-CG	5.55	124.24	113.70	8	3
1	A	79	PHE	CB-CG-CD1	5.54	124.68	120.80	3	1
1	A	39	GLU	OE1-CD-OE2	5.50	129.91	123.30	2	1
1	A	94	PHE	CB-CG-CD1	-5.50	116.95	120.80	3	1
1	A	63	PHE	CB-CG-CD2	-5.46	116.98	120.80	8	1
1	A	34	PHE	CB-CG-CD1	-5.43	117.00	120.80	4	1
1	A	32	ARG	NE-CZ-NH2	-5.43	117.59	120.30	10	2
1	A	35	LYS	O-C-N	-5.37	114.11	122.70	6	1
1	A	53	TYR	CA-CB-CG	5.37	123.60	113.40	10	2
1	A	14	TYR	CB-CG-CD1	5.35	124.21	121.00	9	2
1	A	34	PHE	CB-CG-CD2	-5.27	117.11	120.80	9	1
1	A	29	GLU	CG-CD-OE1	5.26	128.81	118.30	2	1
1	A	41	GLN	CG-CD-OE1	5.19	131.97	121.60	2	1
1	A	9	GLU	OE1-CD-OE2	-5.13	117.15	123.30	2	1
1	A	108	LEU	CB-CA-C	5.07	119.83	110.20	6	1

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	987	972	972	10±7
2	A	33	42	41	3±5
3	A	32	42	41	3±2
All	All	10520	10560	10556	107

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:TYR:CZ	1:A:57:HIS:HB3	1.23	1.68	1	1
1:A:53:TYR:CE2	1:A:57:HIS:HB3	1.17	1.72	1	1
1:A:53:TYR:CZ	1:A:57:HIS:CB	1.04	2.40	1	1
1:A:123:SER:CB	2:A:201:GCH:H32	1.00	1.85	10	1
1:A:123:SER:CB	2:A:201:GCH:H36	0.88	1.98	10	2
1:A:53:TYR:OH	1:A:57:HIS:CB	0.86	2.23	1	1
1:A:97:TYR:OH	3:A:202:CHO:C21	0.86	2.24	2	1
1:A:123:SER:HB3	2:A:201:GCH:H36	0.85	1.45	10	1
1:A:123:SER:HB3	2:A:201:GCH:H32	0.84	1.49	10	1
1:A:123:SER:HB2	2:A:201:GCH:H32	0.82	1.51	10	1
1:A:53:TYR:OH	1:A:57:HIS:CG	0.81	2.32	1	1
1:A:47:PHE:CD2	1:A:63:PHE:CE1	0.79	2.71	1	1
1:A:73:THR:HB	3:A:202:CHO:C27	0.79	2.08	10	1
1:A:97:TYR:CD1	1:A:114:ILE:HG12	0.78	2.13	4	2
1:A:97:TYR:OH	3:A:202:CHO:H212	0.78	1.78	2	1
1:A:63:PHE:CZ	3:A:202:CHO:H5	0.74	2.18	1	2
1:A:21:LEU:HD22	1:A:97:TYR:CE1	0.69	2.23	9	1
1:A:53:TYR:CE2	1:A:57:HIS:CB	0.67	2.66	1	1
1:A:53:TYR:OH	1:A:57:HIS:ND1	0.65	2.30	1	1
1:A:49:TRP:CH2	3:A:202:CHO:H14	0.64	2.26	9	1
1:A:108:LEU:HD21	2:A:201:GCH:H37	0.63	1.71	9	1
1:A:123:SER:OG	2:A:201:GCH:C23	0.62	2.48	10	1
1:A:123:SER:CB	2:A:201:GCH:C23	0.61	2.77	10	1
1:A:11:GLU:HB3	1:A:14:TYR:CD1	0.60	2.31	7	1
2:A:201:GCH:H38	2:A:201:GCH:H21	0.59	1.75	2	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:TYR:CE1	1:A:114:ILE:CG1	0.58	2.86	4	1
1:A:73:THR:CB	3:A:202:CHO:C27	0.58	2.82	10	1
1:A:97:TYR:CD1	1:A:114:ILE:CG1	0.57	2.86	4	1
1:A:73:THR:HG22	1:A:79:PHE:CZ	0.57	2.35	8	2
1:A:63:PHE:CE2	1:A:83:VAL:HG21	0.57	2.35	1	1
1:A:38:THR:CG2	2:A:201:GCH:H41	0.56	2.30	9	1
1:A:49:TRP:CD2	3:A:202:CHO:O7	0.56	2.58	9	1
1:A:97:TYR:OH	1:A:112:SER:OG	0.56	2.23	4	1
1:A:63:PHE:CE1	3:A:202:CHO:C6	0.56	2.89	1	2
1:A:97:TYR:CE1	1:A:114:ILE:HG12	0.55	2.35	4	1
1:A:38:THR:HG23	2:A:201:GCH:H41	0.55	1.78	9	1
1:A:21:LEU:CD2	1:A:97:TYR:CE1	0.55	2.90	9	2
1:A:30:LYS:HE2	1:A:53:TYR:CD2	0.54	2.37	9	1
1:A:73:THR:HA	3:A:202:CHO:H181	0.54	1.80	6	1
1:A:40:VAL:HG21	2:A:201:GCH:C5	0.54	2.33	4	1
1:A:123:SER:OG	2:A:201:GCH:H36	0.54	2.03	10	1
1:A:97:TYR:OH	3:A:202:CHO:C20	0.53	2.56	2	1
1:A:49:TRP:CE3	3:A:202:CHO:H41	0.52	2.38	9	1
2:A:201:GCH:H38	2:A:201:GCH:C19	0.52	2.35	2	1
1:A:97:TYR:OH	3:A:202:CHO:H121	0.51	2.06	9	1
1:A:90:LEU:HB2	3:A:202:CHO:H22	0.50	1.82	4	1
1:A:17:PHE:CE2	1:A:119:TYR:CD2	0.50	3.00	3	1
1:A:1:ALA:HA	1:A:42:GLN:OE1	0.50	2.07	2	2
1:A:14:TYR:CD2	1:A:15:ASP:N	0.50	2.79	7	1
1:A:63:PHE:CZ	3:A:202:CHO:C5	0.50	2.95	1	1
1:A:38:THR:HG21	2:A:201:GCH:H41	0.49	1.83	7	1
1:A:5:LYS:H	1:A:127:ALA:HB2	0.49	1.68	7	1
1:A:63:PHE:CE1	3:A:202:CHO:H5	0.48	2.43	4	1
1:A:121:ARG:HE	2:A:201:GCH:H30	0.48	1.68	2	1
1:A:121:ARG:HD3	2:A:201:GCH:H31	0.48	1.86	1	1
1:A:49:TRP:CE3	3:A:202:CHO:O7	0.48	2.62	9	1
1:A:21:LEU:HD21	1:A:97:TYR:CE1	0.48	2.44	4	1
1:A:108:LEU:HB3	2:A:201:GCH:H15	0.47	1.86	10	1
1:A:53:TYR:HH	1:A:57:HIS:CG	0.47	2.14	1	1
1:A:121:ARG:HD3	2:A:201:GCH:H26	0.47	1.85	10	1
1:A:6:PHE:CD1	1:A:108:LEU:HD21	0.47	2.44	8	1
2:A:201:GCH:H38	2:A:201:GCH:H20	0.47	1.86	5	1
1:A:8:MET:SD	2:A:201:GCH:N	0.46	2.86	10	1
1:A:47:PHE:CE2	1:A:63:PHE:CE1	0.46	3.04	1	1
1:A:49:TRP:CZ3	3:A:202:CHO:H41	0.46	2.46	9	1
1:A:97:TYR:HD1	1:A:114:ILE:HG12	0.46	1.67	4	2

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:MET:N	2:A:201:GCH:H19	0.45	2.27	10	1
1:A:71:ILE:HG23	3:A:202:CHO:H191	0.45	1.89	7	1
1:A:75:GLY:N	3:A:202:CHO:OT1	0.45	2.48	6	1
1:A:8:MET:N	2:A:201:GCH:C19	0.45	2.80	10	1
1:A:108:LEU:HD11	2:A:201:GCH:H18	0.45	1.89	9	1
1:A:108:LEU:CD2	2:A:201:GCH:H37	0.44	2.42	9	1
1:A:21:LEU:HD23	3:A:202:CHO:C24	0.44	2.43	9	1
1:A:107:LYS:C	1:A:108:LEU:HD22	0.44	2.33	10	1
1:A:40:VAL:CG2	2:A:201:GCH:H5	0.43	2.43	4	1
1:A:97:TYR:CE1	1:A:114:ILE:HG13	0.43	2.48	4	1
1:A:10:SER:CB	1:A:122:VAL:H	0.43	2.26	6	2
1:A:53:TYR:OH	1:A:57:HIS:HB2	0.43	2.10	1	1
1:A:11:GLU:CB	1:A:14:TYR:CD1	0.43	3.01	7	1
1:A:2:PHE:CG	2:A:201:GCH:H12	0.43	2.48	1	1
2:A:201:GCH:C23	2:A:201:GCH:C19	0.43	2.97	2	1
1:A:123:SER:HB2	2:A:201:GCH:C16	0.43	2.35	10	1
1:A:99:GLN:OE1	3:A:202:CHO:C12	0.42	2.67	3	1
1:A:97:TYR:CZ	3:A:202:CHO:H20	0.42	2.49	2	1
1:A:108:LEU:HD21	2:A:201:GCH:H7	0.42	1.91	9	1
1:A:10:SER:HB3	1:A:122:VAL:H	0.42	1.74	6	1
1:A:123:SER:OG	2:A:201:GCH:H38	0.42	2.15	10	1
1:A:110:GLU:OE2	1:A:112:SER:HB2	0.41	2.15	8	1
1:A:114:ILE:HD13	1:A:115:GLY:N	0.41	2.29	3	1
1:A:47:PHE:HD2	1:A:63:PHE:CE1	0.41	2.24	1	1
1:A:99:GLN:CD	3:A:202:CHO:H112	0.41	2.35	9	1
1:A:53:TYR:CZ	1:A:57:HIS:HB2	0.41	2.43	1	1
1:A:8:MET:HB2	2:A:201:GCH:H27	0.41	1.92	10	1
1:A:97:TYR:HE1	1:A:114:ILE:HG13	0.41	1.76	4	1
1:A:17:PHE:CZ	1:A:112:SER:HB3	0.41	2.51	8	1
1:A:47:PHE:CB	1:A:63:PHE:CE1	0.41	3.04	4	1
1:A:38:THR:HG23	2:A:201:GCH:C11	0.41	2.45	9	1
1:A:99:GLN:OE1	3:A:202:CHO:H122	0.40	2.17	3	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	122/127 (96%)	111±1 (91±1%)	9±2 (8±1%)	2±1 (1±1%)	18	63
All	All	1220/1270 (96%)	1110 (91%)	92 (8%)	18 (1%)	18	63

All 11 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	35	LYS	7
1	A	3	THR	2
1	A	33	ASN	1
1	A	10	SER	1
1	A	13	ASN	1
1	A	11	GLU	1
1	A	22	GLY	1
1	A	57	HIS	1
1	A	26	ASP	1
1	A	36	ILE	1
1	A	53	TYR	1

### 6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	109/110 (99%)	95±3 (87±3%)	14±3 (13±3%)	9	51
All	All	1090/1100 (99%)	949 (87%)	141 (13%)	9	51

All 50 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	126	LEU	10
1	A	100	THR	8
1	A	91	VAL	8
1	A	5	LYS	8
1	A	79	PHE	8
1	A	49	TRP	7
1	A	80	LYS	5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	117	VAL	5
1	A	59	MET	4
1	A	99	GLN	4
1	A	65	VAL	4
1	A	35	LYS	4
1	A	112	SER	4
1	A	114	ILE	4
1	A	101	SER	3
1	A	34	PHE	3
1	A	119	TYR	3
1	A	118	THR	3
1	A	60	THR	3
1	A	41	GLN	3
1	A	18	MET	2
1	A	38	THR	2
1	A	23	ILE	2
1	A	28	ILE	2
1	A	103	ILE	2
1	A	78	THR	2
1	A	84	GLN	2
1	A	124	LYS	2
1	A	21	LEU	2
1	A	70	ASN	2
1	A	47	PHE	1
1	A	9	GLU	1
1	A	61	ASN	1
1	A	110	GLU	1
1	A	106	ASP	1
1	A	68	GLU	1
1	A	121	ARG	1
1	A	13	ASN	1
1	A	11	GLU	1
1	A	85	MET	1
1	A	125	ARG	1
1	A	27	VAL	1
1	A	30	LYS	1
1	A	15	ASP	1
1	A	29	GLU	1
1	A	64	THR	1
1	A	102	GLU	1
1	A	26	ASP	1
1	A	69	SER	1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	57	HIS	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](#)

2 ligands are 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	GCH	A	201	-	33,36,36	1.83±0.20	0±0 (1±1%)
3	CHO	A	202	-	32,35,35	1.74±0.19	0±1 (0±1%)

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	GCH	A	201	-	52,56,56	2.70±0.28	4±2 (7±4%)
3	CHO	A	202	-	50,54,54	2.50±0.35	3±2 (5±3%)

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	GCH	A	201	-	-	0±0,12,79,79	0±0,4,4,4
3	CHO	A	202	-	-	0±0,12,75,75	0±0,4,4,4

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	201	GCH	C13-C12	6.71	1.64	1.54	6	1
2	A	201	GCH	C11-C10	6.34	1.64	1.53	2	1
2	A	201	GCH	C23-C13	5.92	1.64	1.54	9	1
3	A	202	CHO	C6-C7	5.73	1.43	1.52	7	1
2	A	201	GCH	C3-C2	5.30	1.46	1.55	4	1
3	A	202	CHO	C10-C9	5.16	1.46	1.56	7	1

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
3	A	202	CHO	C9-C8-C7	10.46	124.53	111.89	2	3
2	A	201	GCH	C7-C2-C3	8.66	121.95	112.66	1	3
2	A	201	GCH	C7-C2-C1	8.27	102.19	111.07	2	2
2	A	201	GCH	C10-C11-C12	7.88	124.28	114.38	9	2
2	A	201	GCH	C15-C14-C13	7.77	96.10	103.59	8	1
3	A	202	CHO	C6-C5-C4	7.38	103.15	111.07	9	1
3	A	202	CHO	C23-C22-C20	7.34	128.10	114.46	5	3
2	A	201	GCH	C13-C14-C9	7.05	105.46	114.73	9	1
3	A	202	CHO	C14-C8-C9	7.04	99.70	109.63	2	3
2	A	201	GCH	C23-C13-C12	6.80	115.90	109.09	1	1
2	A	201	GCH	C16-C17-C13	6.66	97.17	103.59	10	2
2	A	201	GCH	C4-C3-C2	6.57	115.00	107.76	1	1
2	A	201	GCH	CA-N-C22	6.54	133.52	122.34	10	4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	201	GCH	C14-C9-C10	6.54	100.41	109.63	3	1
3	A	202	CHO	C16-C17-C20	6.47	122.47	112.12	5	2
2	A	201	GCH	C7-C8-C9	6.44	118.28	111.46	9	5
2	A	201	GCH	C16-C17-C18	6.41	122.37	112.12	10	1
2	A	201	GCH	C14-C13-C12	6.39	101.59	107.37	6	1
3	A	202	CHO	C1-C10-C5	6.35	100.77	107.76	2	2
3	A	202	CHO	O7-C7-C8	6.29	123.61	109.28	8	2
3	A	202	CHO	C21-C20-C17	6.24	103.37	112.99	5	4
3	A	202	CHO	C16-C17-C13	6.20	96.56	103.83	10	1
2	A	201	GCH	C2-C7-C8	6.12	121.41	114.44	4	2
3	A	202	CHO	C12-C13-C17	6.06	107.67	116.58	5	2
3	A	202	CHO	C6-C7-C8	6.01	117.83	111.46	6	1
3	A	202	CHO	C4-C3-C2	6.00	102.85	110.53	9	1
2	A	201	GCH	C21-C20-C18	5.91	125.45	114.46	10	1
3	A	202	CHO	C6-C5-C10	5.87	118.96	112.66	9	1
2	A	201	GCH	C10-C3-C2	5.79	116.93	108.68	3	1
2	A	201	GCH	C1-C2-C3	5.73	106.51	112.66	1	2
3	A	202	CHO	C10-C9-C8	5.64	105.75	111.86	5	1
2	A	201	GCH	C17-C13-C14	5.50	94.52	100.08	9	2
2	A	201	GCH	C3-C10-C9	5.49	105.92	111.86	1	1
2	A	201	GCH	C19-C18-C20	5.45	101.47	110.33	7	1
2	A	201	GCH	C19-C18-C17	5.41	121.33	112.99	3	2
3	A	202	CHO	C19-C10-C9	5.27	118.16	111.20	2	1
2	A	201	GCH	C13-C17-C18	5.22	125.80	119.44	9	1

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

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 90% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2mm3\_cs.str

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 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	1564
Number of shifts mapped to atoms	1564
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	127	$-0.54 \pm 0.12$	Should be applied
$^{13}\text{C}_\beta$	114	$-0.30 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	123	$0.24 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	125	$-4.10 \pm 0.44$	Should be applied

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 1373 atoms were assigned a chemical shift out of a possible 1522. 17 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	612/618 (99%)	246/247 (100%)	244/248 (98%)	122/123 (99%)
Sidechain	665/767 (87%)	411/447 (92%)	241/286 (84%)	13/34 (38%)

*Continued on next page...*

Continued from previous page...

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	96/137 (70%)	62/74 (84%)	33/59 (56%)	1/4 (25%)
Overall	1373/1522 (90%)	719/768 (94%)	518/593 (87%)	136/161 (84%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1391 atoms were assigned a chemical shift out of a possible 1540. 17 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	627/633 (99%)	252/253 (100%)	250/254 (98%)	125/126 (99%)
Sidechain	668/770 (87%)	413/449 (92%)	242/287 (84%)	13/34 (38%)
Aromatic	96/137 (70%)	62/74 (84%)	33/59 (56%)	1/4 (25%)
Overall	1391/1540 (90%)	727/776 (94%)	525/600 (88%)	139/164 (85%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 7.1.5 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:

