



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 10:12 pm GMT

PDB ID : 2JGW
Title : STRUCTURE OF CCP MODULE 7 OF COMPLEMENT FACTOR H - THE
AMD AT RISK VARIANT (402H)
Authors : Herbert, A.P.; Deakin, J.A.; Schmidt, C.Q.; Blaum, B.S.; Egan, C.; Ferreira,
V.P.; Pangburn, M.K.; Lyon, M.; Uhrin, D.; Barlow, P.N.
Deposited on : 2007-02-16

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

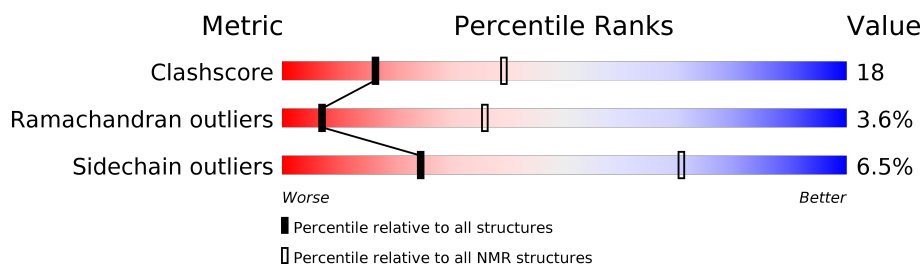
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 88%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	61	

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:387-A:446 (60)	0.46	6

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 4 clusters and 9 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 969 atoms, of which 480 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called COMPLEMENT FACTOR H.

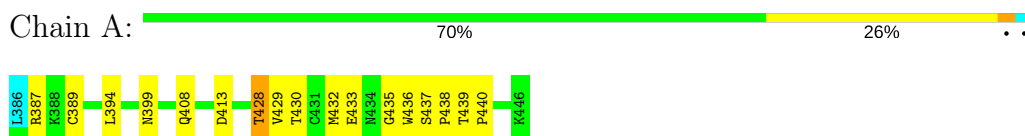
Mol	Chain	Residues	Atoms						Trace
1	A	61	Total	C	H	N	O	S	0
			969	309	480	90	85	5	

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: COMPLEMENT FACTOR H

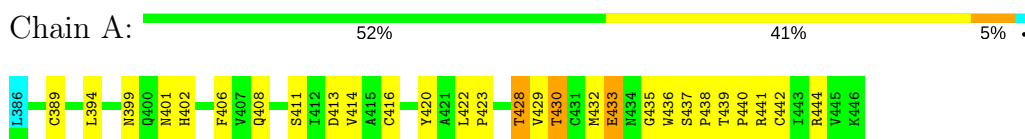


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

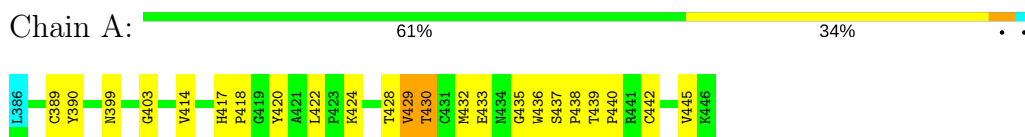
4.2.1 Score per residue for model 1

- Molecule 1: COMPLEMENT FACTOR H



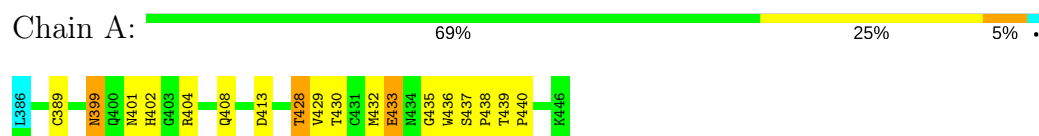
4.2.2 Score per residue for model 2

- Molecule 1: COMPLEMENT FACTOR H



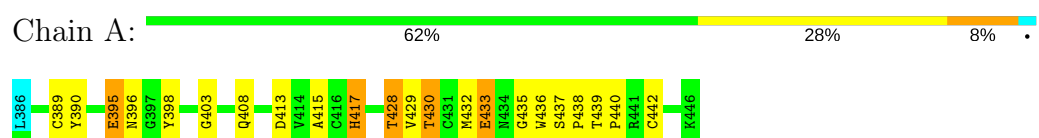
4.2.3 Score per residue for model 3

- Molecule 1: COMPLEMENT FACTOR H



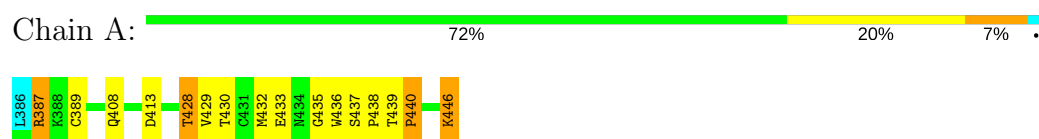
4.2.4 Score per residue for model 4

- Molecule 1: COMPLEMENT FACTOR H



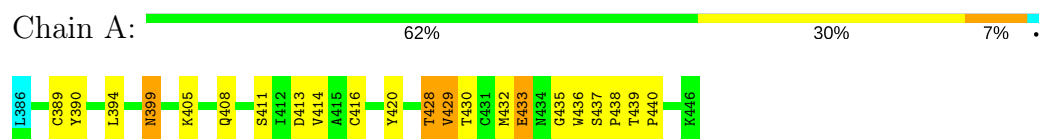
4.2.5 Score per residue for model 5

- Molecule 1: COMPLEMENT FACTOR H



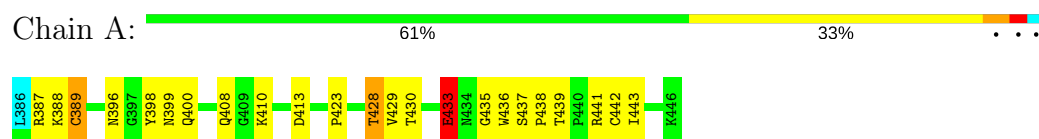
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: COMPLEMENT FACTOR H



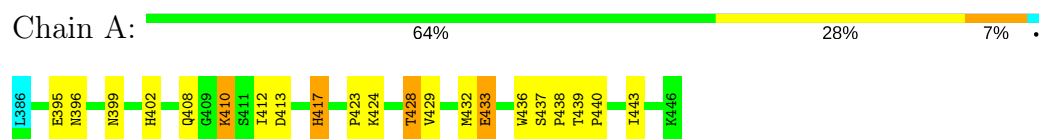
4.2.7 Score per residue for model 7

- Molecule 1: COMPLEMENT FACTOR H



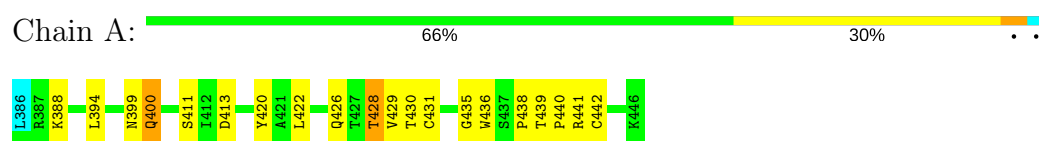
4.2.8 Score per residue for model 8

- Molecule 1: COMPLEMENT FACTOR H



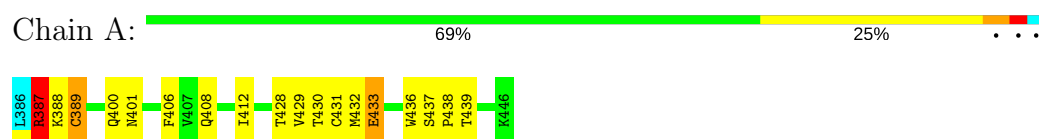
4.2.9 Score per residue for model 9

- Molecule 1: COMPLEMENT FACTOR H



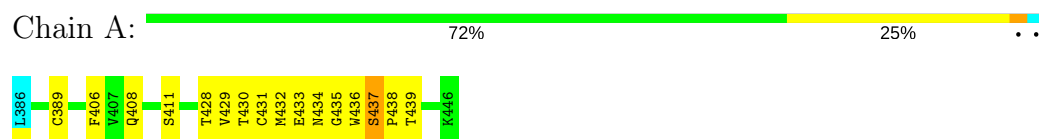
4.2.10 Score per residue for model 10

- Molecule 1: COMPLEMENT FACTOR H



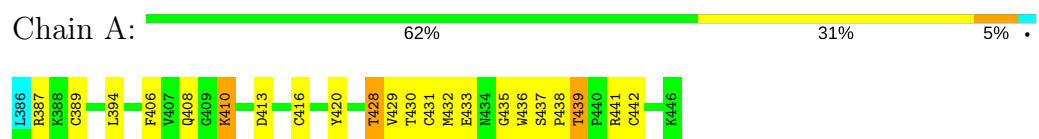
4.2.11 Score per residue for model 11

- Molecule 1: COMPLEMENT FACTOR H



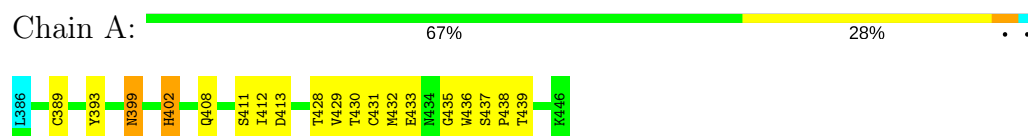
4.2.12 Score per residue for model 12

- Molecule 1: COMPLEMENT FACTOR H



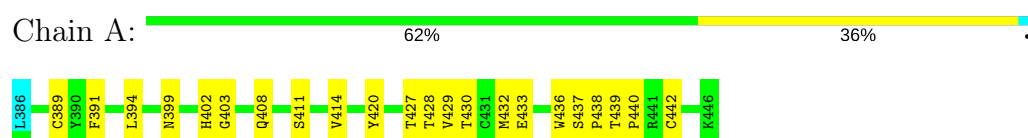
4.2.13 Score per residue for model 13

- Molecule 1: COMPLEMENT FACTOR H



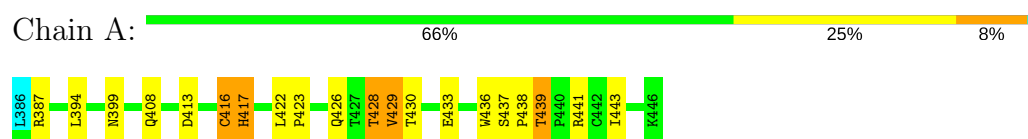
4.2.14 Score per residue for model 14

- Molecule 1: COMPLEMENT FACTOR H



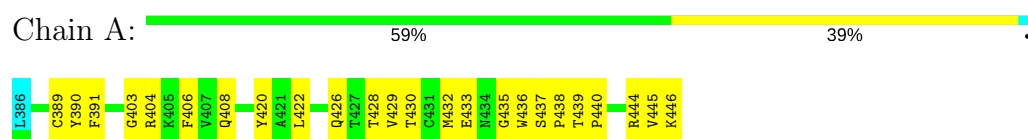
4.2.15 Score per residue for model 15

- Molecule 1: COMPLEMENT FACTOR H



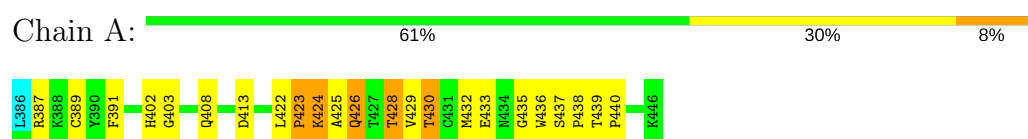
4.2.16 Score per residue for model 16

- Molecule 1: COMPLEMENT FACTOR H



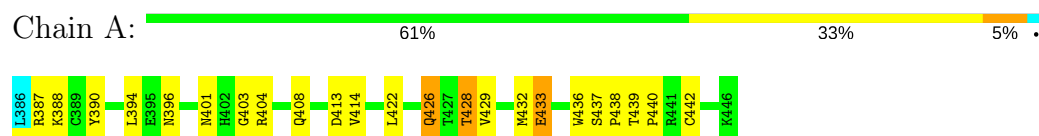
4.2.17 Score per residue for model 17

- Molecule 1: COMPLEMENT FACTOR H



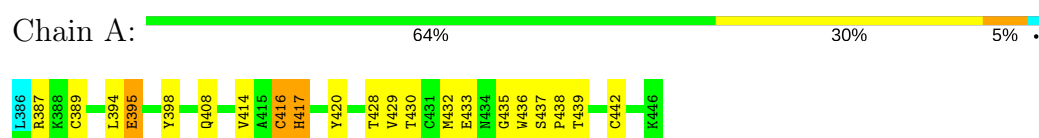
4.2.18 Score per residue for model 18

- Molecule 1: COMPLEMENT FACTOR H



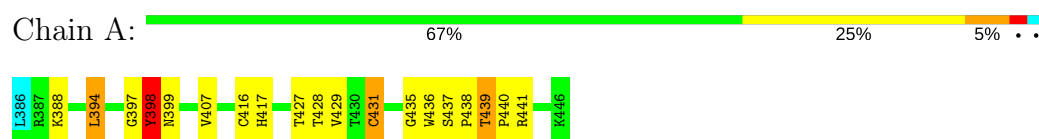
4.2.19 Score per residue for model 19

- Molecule 1: COMPLEMENT FACTOR H



4.2.20 Score per residue for model 20

- Molecule 1: COMPLEMENT FACTOR H



5 Refinement protocol and experimental data overview

The models were refined using the following method: *ARIA 2.0*.

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *LOWEST OVERALL ENERGY*.

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

Software name	Classification	Version
CNS 1.1	refinement	
CCPNMR ANALYSIS	structure solution	

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)	BMRB entry 7420
Number of chemical shift lists	1
Total number of shifts	782
Number of shifts mapped to atoms	749
Number of unparsed shifts	0
Number of shifts with mapping errors	33
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

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

6 Model quality

6.1 Standard geometry

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	481	469	467	17±5
All	All	9620	9380	9340	336

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 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:399:ASN:HB3	1:A:402:HIS:HB2	0.90	1.43	13	2
1:A:389:CYS:SG	1:A:406:PHE:HB2	0.83	2.13	11	2
1:A:406:PHE:HB2	1:A:410:LYS:HE3	0.83	1.50	12	1
1:A:429:VAL:HA	1:A:438:PRO:HG2	0.82	1.52	8	19
1:A:406:PHE:HB3	1:A:410:LYS:HG2	0.77	1.55	12	1
1:A:398:TYR:CD1	1:A:416:CYS:HA	0.76	2.14	20	1
1:A:387:ARG:HA	1:A:408:GLN:HB2	0.74	1.58	5	2
1:A:410:LYS:HA	1:A:410:LYS:HE2	0.74	1.60	7	1
1:A:390:TYR:HA	1:A:405:LYS:HB3	0.74	1.60	6	1
1:A:391:PHE:CZ	1:A:406:PHE:CD2	0.73	2.77	16	1
1:A:422:LEU:HB2	1:A:426:GLN:O	0.73	1.84	17	3
1:A:391:PHE:HZ	1:A:406:PHE:N	0.71	1.83	16	1
1:A:423:PRO:HD2	1:A:425:ALA:HB3	0.70	1.63	17	1
1:A:391:PHE:CD1	1:A:436:TRP:HZ2	0.69	2.05	16	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:410:LYS:HE2	1:A:436:TRP:CH2	0.69	2.23	12	1
1:A:413:ASP:HA	1:A:428:THR:HB	0.68	1.65	13	1
1:A:406:PHE:HB2	1:A:410:LYS:CE	0.67	2.19	12	1
1:A:408:GLN:NE2	1:A:433:GLU:HA	0.66	2.06	16	14
1:A:424:LYS:HE2	1:A:424:LYS:HA	0.66	1.67	2	1
1:A:406:PHE:CB	1:A:410:LYS:HE3	0.66	2.20	12	1
1:A:391:PHE:CD2	1:A:404:ARG:HB2	0.65	2.27	16	1
1:A:391:PHE:HZ	1:A:406:PHE:H	0.65	1.33	16	1
1:A:389:CYS:SG	1:A:435:GLY:HA2	0.65	2.31	1	11
1:A:429:VAL:CG2	1:A:436:TRP:HB3	0.65	2.22	4	19
1:A:401:ASN:HD22	1:A:406:PHE:HZ	0.65	1.35	1	1
1:A:410:LYS:HE3	1:A:410:LYS:HA	0.64	1.70	8	1
1:A:431:CYS:SG	1:A:436:TRP:CZ3	0.64	2.90	10	2
1:A:417:HIS:CG	1:A:418:PRO:HD2	0.63	2.28	2	1
1:A:417:HIS:H	1:A:417:HIS:CD2	0.63	2.10	15	2
1:A:391:PHE:CD1	1:A:436:TRP:CZ2	0.62	2.86	16	1
1:A:437:SER:HB3	1:A:438:PRO:HD3	0.62	1.69	10	10
1:A:437:SER:OG	1:A:438:PRO:HD3	0.62	1.94	5	9
1:A:387:ARG:HB2	1:A:408:GLN:OE1	0.62	1.95	17	1
1:A:394:LEU:HB2	1:A:397:GLY:O	0.61	1.95	20	1
1:A:414:VAL:HB	1:A:422:LEU:HD21	0.61	1.71	18	1
1:A:394:LEU:HD21	1:A:441:ARG:HA	0.60	1.73	9	1
1:A:394:LEU:CD2	1:A:441:ARG:HA	0.58	2.28	9	1
1:A:413:ASP:HA	1:A:428:THR:HA	0.58	1.76	1	12
1:A:391:PHE:CZ	1:A:406:PHE:N	0.58	2.71	16	1
1:A:410:LYS:HE2	1:A:436:TRP:CZ3	0.58	2.32	12	1
1:A:417:HIS:CD2	1:A:417:HIS:H	0.58	2.14	8	1
1:A:398:TYR:HE2	1:A:416:CYS:CA	0.58	2.11	19	1
1:A:420:TYR:HB3	1:A:442:CYS:HB3	0.58	1.75	19	4
1:A:391:PHE:CE2	1:A:406:PHE:CD2	0.58	2.92	16	1
1:A:413:ASP:HA	1:A:428:THR:CB	0.58	2.28	13	1
1:A:422:LEU:HB2	1:A:426:GLN:HB2	0.57	1.75	9	1
1:A:391:PHE:N	1:A:391:PHE:CD1	0.57	2.64	16	1
1:A:429:VAL:HG23	1:A:438:PRO:HD2	0.57	1.75	16	17
1:A:429:VAL:HG11	1:A:440:PRO:HB3	0.57	1.76	16	1
1:A:424:LYS:O	1:A:426:GLN:HG3	0.57	2.00	17	1
1:A:387:ARG:CA	1:A:408:GLN:HB2	0.56	2.30	5	1
1:A:430:THR:O	1:A:436:TRP:HA	0.56	2.00	14	16
1:A:398:TYR:OH	1:A:414:VAL:HG13	0.56	2.01	19	1
1:A:408:GLN:HE21	1:A:433:GLU:HA	0.55	1.62	11	3
1:A:417:HIS:CD2	1:A:418:PRO:HD2	0.55	2.36	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:391:PHE:HZ	1:A:414:VAL:HG22	0.55	1.62	14	1
1:A:414:VAL:HB	1:A:422:LEU:HD11	0.55	1.79	1	2
1:A:432:MET:HG2	1:A:435:GLY:O	0.55	2.01	16	6
1:A:399:ASN:O	1:A:400:GLN:HG2	0.55	2.01	9	1
1:A:390:TYR:CE1	1:A:403:GLY:HA2	0.54	2.36	16	3
1:A:420:TYR:CE2	1:A:444:ARG:HB2	0.54	2.37	16	1
1:A:429:VAL:HG21	1:A:440:PRO:HG3	0.54	1.80	2	1
1:A:390:TYR:HA	1:A:405:LYS:CB	0.54	2.30	6	1
1:A:429:VAL:HG22	1:A:436:TRP:CE3	0.54	2.38	12	5
1:A:436:TRP:CB	1:A:440:PRO:HD3	0.53	2.33	4	12
1:A:389:CYS:SG	1:A:406:PHE:CB	0.53	2.95	11	2
1:A:398:TYR:N	1:A:398:TYR:CD1	0.53	2.77	20	1
1:A:388:LYS:HG2	1:A:407:VAL:HG23	0.53	1.80	20	1
1:A:408:GLN:HA	1:A:431:CYS:SG	0.53	2.44	13	2
1:A:398:TYR:CE2	1:A:416:CYS:N	0.53	2.77	19	1
1:A:398:TYR:CE2	1:A:416:CYS:CA	0.52	2.91	19	1
1:A:399:ASN:CB	1:A:402:HIS:HB2	0.52	2.34	1	1
1:A:398:TYR:N	1:A:398:TYR:CD2	0.52	2.71	19	1
1:A:425:ALA:O	1:A:426:GLN:HB2	0.52	2.05	17	1
1:A:391:PHE:CE2	1:A:404:ARG:C	0.51	2.84	16	1
1:A:398:TYR:HE2	1:A:416:CYS:HA	0.51	1.66	19	1
1:A:398:TYR:CE2	1:A:416:CYS:HA	0.51	2.40	19	1
1:A:394:LEU:HD23	1:A:416:CYS:SG	0.50	2.46	15	1
1:A:445:VAL:O	1:A:446:LYS:HB2	0.50	2.06	16	1
1:A:432:MET:HB3	1:A:437:SER:HB3	0.50	1.83	11	8
1:A:432:MET:SD	1:A:437:SER:HB3	0.50	2.47	1	6
1:A:394:LEU:HD23	1:A:442:CYS:SG	0.49	2.47	18	3
1:A:423:PRO:HA	1:A:443:ILE:HD11	0.49	1.84	7	3
1:A:399:ASN:HB2	1:A:402:HIS:HB2	0.49	1.84	8	2
1:A:399:ASN:HB3	1:A:402:HIS:CB	0.49	2.29	13	1
1:A:424:LYS:HE2	1:A:438:PRO:HA	0.49	1.84	8	1
1:A:410:LYS:HZ3	1:A:431:CYS:HB2	0.49	1.68	12	1
1:A:389:CYS:HB3	1:A:435:GLY:HA2	0.49	1.85	7	1
1:A:396:ASN:OD1	1:A:442:CYS:HB2	0.49	2.08	7	1
1:A:400:GLN:HG3	1:A:401:ASN:OD1	0.49	2.08	10	1
1:A:432:MET:HG3	1:A:433:GLU:N	0.48	2.23	5	9
1:A:446:LYS:HB3	1:A:446:LYS:NZ	0.48	2.23	5	1
1:A:387:ARG:HB2	1:A:408:GLN:NE2	0.48	2.24	12	1
1:A:396:ASN:HB2	1:A:417:HIS:ND1	0.48	2.24	4	2
1:A:432:MET:HB3	1:A:437:SER:HB2	0.48	1.84	10	1
1:A:387:ARG:O	1:A:387:ARG:HG3	0.48	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:439:THR:O	1:A:441:ARG:HG2	0.48	2.09	12	2
1:A:410:LYS:HD2	1:A:431:CYS:CB	0.48	2.39	12	1
1:A:416:CYS:SG	1:A:420:TYR:HB2	0.48	2.49	6	3
1:A:394:LEU:HD13	1:A:442:CYS:H	0.47	1.69	9	1
1:A:441:ARG:HG3	1:A:441:ARG:O	0.47	2.09	9	1
1:A:423:PRO:HD3	1:A:441:ARG:O	0.46	2.10	7	2
1:A:394:LEU:HG	1:A:398:TYR:CE2	0.46	2.45	20	1
1:A:391:PHE:O	1:A:402:HIS:ND1	0.45	2.49	14	2
1:A:439:THR:HG22	1:A:441:ARG:HG2	0.45	1.88	20	1
1:A:410:LYS:CE	1:A:431:CYS:HB2	0.45	2.40	12	1
1:A:389:CYS:HB2	1:A:410:LYS:NZ	0.45	2.26	12	1
1:A:429:VAL:HG21	1:A:436:TRP:HB3	0.45	1.87	13	2
1:A:422:LEU:HB2	1:A:426:GLN:HB3	0.45	1.87	18	1
1:A:420:TYR:HA	1:A:444:ARG:HA	0.45	1.89	1	1
1:A:398:TYR:HB2	1:A:415:ALA:HB3	0.45	1.88	4	1
1:A:394:LEU:HB3	1:A:417:HIS:CE1	0.44	2.47	19	1
1:A:417:HIS:N	1:A:417:HIS:CD2	0.44	2.85	8	2
1:A:398:TYR:HB3	1:A:400:GLN:OE1	0.44	2.12	7	1
1:A:422:LEU:HD13	1:A:425:ALA:O	0.44	2.12	17	1
1:A:394:LEU:HD11	1:A:440:PRO:HB2	0.44	1.89	14	1
1:A:394:LEU:HB3	1:A:417:HIS:HE1	0.44	1.72	19	1
1:A:394:LEU:H	1:A:399:ASN:ND2	0.44	2.10	6	1
1:A:431:CYS:SG	1:A:435:GLY:HA2	0.44	2.53	20	2
1:A:391:PHE:CE2	1:A:404:ARG:HB2	0.43	2.47	16	1
1:A:393:TYR:HA	1:A:402:HIS:CD2	0.43	2.48	13	1
1:A:414:VAL:HG21	1:A:440:PRO:HB3	0.43	1.90	6	1
1:A:390:TYR:CA	1:A:405:LYS:HB3	0.43	2.40	6	1
1:A:411:SER:OG	1:A:430:THR:HG22	0.43	2.14	14	4
1:A:391:PHE:HD2	1:A:404:ARG:HB2	0.42	1.68	16	1
1:A:423:PRO:HD2	1:A:425:ALA:CB	0.42	2.42	17	1
1:A:411:SER:HA	1:A:430:THR:HB	0.42	1.90	1	1
1:A:429:VAL:HG23	1:A:436:TRP:CE3	0.42	2.50	2	1
1:A:401:ASN:HA	1:A:404:ARG:HD2	0.42	1.91	3	1
1:A:401:ASN:CB	1:A:404:ARG:HD2	0.41	2.46	18	1
1:A:406:PHE:CB	1:A:410:LYS:HG2	0.41	2.39	12	1
1:A:402:HIS:CG	1:A:403:GLY:N	0.41	2.88	14	2
1:A:417:HIS:CG	1:A:418:PRO:CD	0.41	3.03	2	1
1:A:406:PHE:HB2	1:A:410:LYS:NZ	0.41	2.29	12	1
1:A:389:CYS:HB2	1:A:410:LYS:HZ3	0.41	1.76	12	1
1:A:422:LEU:HB3	1:A:425:ALA:HB3	0.41	1.92	17	1
1:A:410:LYS:NZ	1:A:431:CYS:HB2	0.41	2.30	12	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:436:TRP:HB3	1:A:440:PRO:HD3	0.41	1.91	20	2
1:A:436:TRP:HB2	1:A:440:PRO:HD3	0.41	1.92	4	1
1:A:411:SER:CB	1:A:430:THR:HG22	0.40	2.46	13	1
1:A:390:TYR:CZ	1:A:403:GLY:HA2	0.40	2.51	2	1
1:A:410:LYS:CE	1:A:436:TRP:CH2	0.40	3.02	12	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	59/61 (97%)	50±2 (84±3%)	7±2 (12±3%)	2±1 (4±1%)	7	36
All	All	1180/1220 (97%)	993 (84%)	144 (12%)	43 (4%)	7	36

All 14 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	439	THR	20
1	A	433	GLU	9
1	A	395	GLU	3
1	A	387	ARG	1
1	A	423	PRO	1
1	A	426	GLN	1
1	A	445	VAL	1
1	A	388	LYS	1
1	A	442	CYS	1
1	A	398	TYR	1
1	A	400	GLN	1
1	A	416	CYS	1
1	A	440	PRO	1
1	A	412	ILE	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	52/53 (98%)	49±2 (93±3%)	3±2 (7±3%)	24 71
All	All	1040/1060 (98%)	972 (93%)	68 (7%)	24 71

All 23 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	428	THR	19
1	A	399	ASN	8
1	A	417	HIS	5
1	A	387	ARG	5
1	A	430	THR	4
1	A	389	CYS	3
1	A	429	VAL	3
1	A	427	THR	2
1	A	388	LYS	2
1	A	410	LYS	2
1	A	412	ILE	2
1	A	395	GLU	2
1	A	446	LYS	1
1	A	424	LYS	1
1	A	426	GLN	1
1	A	398	TYR	1
1	A	416	CYS	1
1	A	394	LEU	1
1	A	396	ASN	1
1	A	433	GLU	1
1	A	437	SER	1
1	A	431	CYS	1
1	A	402	HIS	1

6.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 88% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 7420

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	782
Number of shifts mapped to atoms	749
Number of unparsed shifts	0
Number of shifts with mapping errors	33
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- Residue not found in structure. All 33 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	3	ALA	HB1	1.375	0.005	1
A	3	ALA	HB2	1.375	0.005	1
A	1	GLU	CG	35.58	0.038	1
A	2	ALA	HA	4.303	0.021	1
A	2	ALA	HB1	1.375	0.01	1
A	3	ALA	CB	19.177	0.044	1
A	3	ALA	N	124.323	0.018	1
A	2	ALA	H	8.756	0.004	1
A	1	GLU	HA	4.005	0.006	1
A	1	GLU	CB	30.268	0.058	1
A	3	ALA	H	8.49	0.003	1
A	2	ALA	CB	19.139	0.042	1
A	3	ALA	HA	4.24	0.026	1
A	1	GLU	HG3	2.343	0.013	1

Continued on next page...

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	1	GLU	HB2	2.073	0.01	1
A	1	GLU	HG2	2.343	0.013	1
A	4	GLY	N	107.436	0.035	1
A	2	ALA	HB3	1.375	0.01	1
A	2	ALA	CA	52.533	0.022	1
A	4	GLY	HA2	3.88	0.007	2
A	3	ALA	HB3	1.375	0.005	1
A	1	GLU	HB3	2.073	0.01	1
A	4	GLY	C	174.05	0.007	1
A	4	GLY	H	8.375	0.006	1
A	2	ALA	HB2	1.375	0.01	1
A	3	ALA	CA	53.0	0.05	1
A	2	ALA	C	177.235	0.004	1
A	1	GLU	C	172.394	0.009	1
A	1	GLU	CA	55.533	0.034	1
A	4	GLY	HA3	3.896	0.01	2
A	4	GLY	CA	45.334	0.031	1
A	2	ALA	N	126.618	0.028	1
A	3	ALA	C	178.464	0.001	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	64	0.07 ± 0.25	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	58	0.06 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}'$	56	0.19 ± 0.34	None needed (< 0.5 ppm)
^{15}N	56	-0.66 ± 0.35	None needed (imprecise)

7.1.3 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 88%, i.e. 670 atoms were assigned a chemical shift out of a possible 761. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	273/290 (94%)	111/115 (97%)	110/120 (92%)	52/55 (95%)
Sidechain	338/393 (86%)	213/236 (90%)	114/133 (86%)	11/24 (46%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	59/78 (76%)	31/40 (78%)	27/33 (82%)	1/5 (20%)
Overall	670/761 (88%)	355/391 (91%)	251/286 (88%)	64/84 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 684 atoms were assigned a chemical shift out of a possible 775. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	278/295 (94%)	113/117 (97%)	112/122 (92%)	53/56 (95%)
Sidechain	347/402 (86%)	218/241 (90%)	118/137 (86%)	11/24 (46%)
Aromatic	59/78 (76%)	31/40 (78%)	27/33 (82%)	1/5 (20%)
Overall	684/775 (88%)	362/398 (91%)	257/292 (88%)	65/85 (76%)

7.1.4 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	392	PRO	HD2	1.54	5.45 – 1.85	-5.9

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:

