



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 7, 2026 – 02:56 AM UTC

PDB ID : 6BHN / pdb_00006bhn
BMRB ID : 26582
Title : Red Light-Absorbing State of NpR6012g4, a Red/Green Cyanobacteriochrome
Authors : Yu, Q.; Lim, S.; Rockwell, N.C.; Martin, S.S.; Lagarias, J.C.; Ames, J.B.
Deposited on : 2017-10-31

This is a wwPDB NMR Structure Validation Summary 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

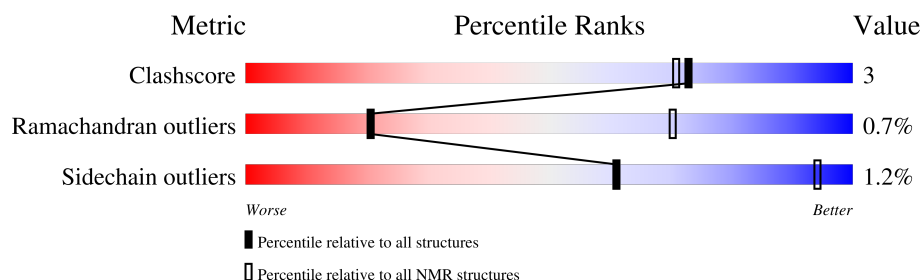
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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	180	

2 Ensemble composition and analysis

This entry contains 10 models. Model 5 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:600-A:643, A:653-A:749 (141)	0.79	5

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 and 4 single-model clusters were found.

Cluster number	Models
1	4, 5
2	3, 6
3	7, 8
Single-model clusters	1; 2; 9; 10

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2552 atoms, of which 1248 are hydrogens and 0 are deuteriums.

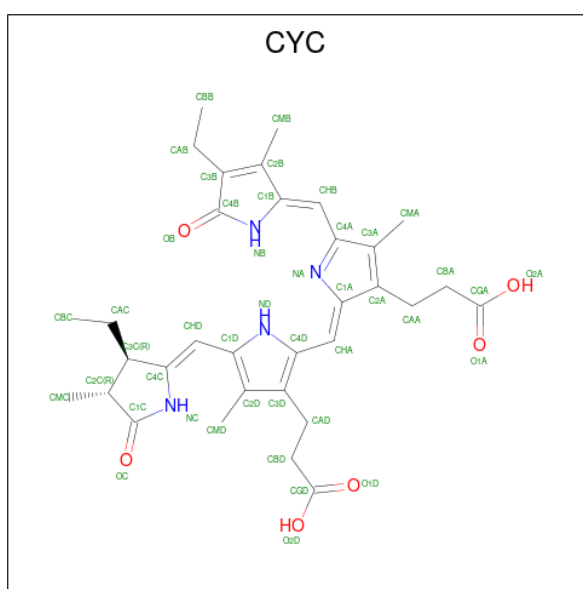
- Molecule 1 is a protein called Methyl-accepting chemotaxis sensory transducer with phytochrome sensor.

Mol	Chain	Residues	Atoms						Trace
1	A	156	Total	C	H	N	O	S	0
			2471	803	1210	214	242	2	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	583	MET	-	initiating methionine	UNP B2IU14
A	584	GLY	-	expression tag	UNP B2IU14
A	761	PRO	-	expression tag	UNP B2IU14
A	762	GLY	-	expression tag	UNP B2IU14

- Molecule 2 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms					
2	A	1	Total	C	H	N	O	
			81	33	38	4	6	

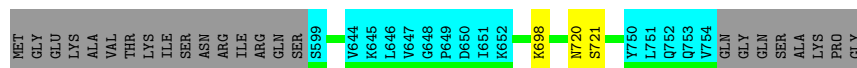
4 Residue-property plots [i](#)

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: Methyl-accepting chemotaxis sensory transducer with phytochrome sensor

Chain A: 

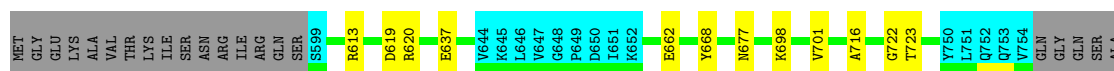


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 5. Colouring as in section 4.1 above.

- Molecule 1: Methyl-accepting chemotaxis sensory transducer with phytochrome sensor

Chain A: 



LYS
PRO
GLY

5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 200 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
X-PLOR NIH	refinement	2.44
NMRPipe	structure solution	8.9
Sparky	structure solution	3.12

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2104
Number of shifts mapped to atoms	1938
Number of unparsed shifts	0
Number of shifts with mapping errors	166
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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 [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	1143	1080	1080	6±1
2	A	43	38	37	2±1
All	All	11860	11180	11170	77

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 3.

5 of 50 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:684:HIS:ND1	1:A:689:ILE:HB	0.64	2.07	8	1
2:A:800:CYC:CHD	2:A:800:CYC:HBC3	0.61	2.26	5	6
1:A:613:ARG:HA	1:A:618:CYS:SG	0.58	2.38	3	2
1:A:677:ASN:O	1:A:723:THR:HA	0.56	2.00	5	2
1:A:657:ASP:O	1:A:661:GLN:HB2	0.54	2.02	4	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	141/180 (78%)	135±1 (96±1%)	5±1 (3±1%)	1±1 (1±1%)	20	70
All	All	1410/1800 (78%)	1352 (96%)	48 (3%)	10 (1%)	20	70

All 3 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	720	ASN	5
1	A	721	SER	3
1	A	686	PRO	2

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	121/154 (79%)	120±2 (99±1%)	2±2 (1±1%)	61	94
All	All	1210/1540 (79%)	1195 (99%)	15 (1%)	61	94

5 of 12 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	730	GLU	2
1	A	617	ARG	2
1	A	637	GLU	2
1	A	600	ASP	1
1	A	667	ARG	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	CYC	A	800	1	46,46,46	1.96±0.06	9±1 (19±3%)

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	CYC	A	800	1	63,67,67	2.41±0.05	19±1 (30±1%)

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	CYC	A	800	1	-	0±0,26,74,74	0±0,4,4,4

5 of 14 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	800	CYC	C1A-NA	7.60	1.54	1.38	7	10
2	A	800	CYC	C4A-C3A	6.04	1.32	1.45	6	10
2	A	800	CYC	C1B-C2B	4.86	1.53	1.45	7	10
2	A	800	CYC	C4A-NA	3.68	1.45	1.36	7	10
2	A	800	CYC	CHB-C4A	3.44	1.48	1.40	4	1

5 of 24 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

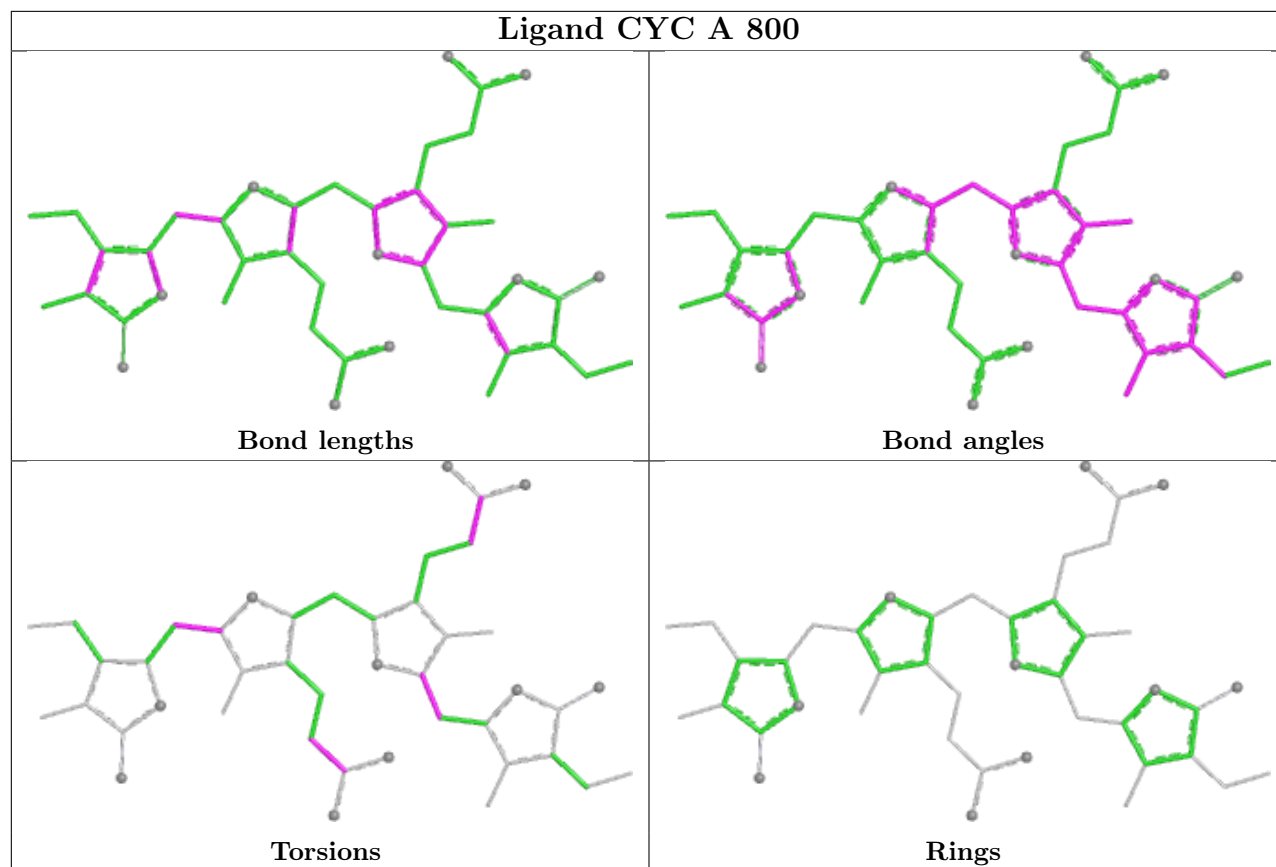
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	800	CYC	C4A-C3A-C2A	9.42	117.17	106.48	7	10
2	A	800	CYC	C2A-C1A-NA	8.15	98.51	110.04	3	10
2	A	800	CYC	C2B-C1B-NB	5.52	98.92	106.97	7	10
2	A	800	CYC	CMB-C2B-C1B	5.28	117.73	124.16	7	9
2	A	800	CYC	C1A-C2A-C3A	5.06	112.21	106.73	8	10

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

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 87% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

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	2104
Number of shifts mapped to atoms	1938
Number of unparsed shifts	0
Number of shifts with mapping errors	166
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	14

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

- No matching atom found in the structure. First 5 (of 166) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	583	MET	C	177.475	0	1
1	A	583	MET	CA	63.18	0.087	1
1	A	583	MET	CB	32.158	0.023	1
1	A	584	GLY	H	8.509	0.021	1
1	A	584	GLY	HA2	4.064	0	2
1	A	584	GLY	HA3	4.064	0	2
1	A	584	GLY	C	173.026	0	1
1	A	584	GLY	CA	44.207	0	1
1	A	584	GLY	N	108.852	0.007	1
1	A	585	GLU	H	8.175	0	1
1	A	585	GLU	HA	4.318	0.012	1
1	A	585	GLU	HB2	1.99	0.009	2
1	A	585	GLU	HB3	1.99	0.009	2
1	A	585	GLU	HG2	2.288	0.002	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	585	GLU	HG3	2.288	0.002	2
1	A	585	GLU	C	176.775	0	1
1	A	585	GLU	CA	56.755	0.007	1
1	A	585	GLU	CB	30.635	0.037	1
1	A	585	GLU	CG	36.151	0	1
1	A	585	GLU	N	119.09	0	1
1	A	586	LYS	H	8.552	0	1
1	A	586	LYS	HA	4.327	0	1
1	A	586	LYS	HB2	1.476	0	2
1	A	586	LYS	HB3	1.796	0	2
1	A	586	LYS	C	176.556	0	1
1	A	586	LYS	CA	56.694	0.015	1
1	A	586	LYS	CB	32.965	0	1
1	A	586	LYS	N	122.682	0	1
1	A	587	ALA	H	8.394	0.011	1
1	A	587	ALA	HA	4.335	0.015	1
1	A	587	ALA	HB1	1.424	0.01	1
1	A	587	ALA	HB2	1.424	0.01	1
1	A	587	ALA	HB3	1.424	0.01	1
1	A	587	ALA	C	178.097	0	1
1	A	587	ALA	CA	53.121	0.014	1
1	A	587	ALA	CB	19.335	0.028	1
1	A	587	ALA	N	125.381	0	1
1	A	588	VAL	H	8.209	0.007	1
1	A	588	VAL	HA	4.133	0.008	1
1	A	588	VAL	HB	2.087	0.021	1
1	A	588	VAL	HG11	0.931	0.017	1
1	A	588	VAL	HG12	0.931	0.017	1
1	A	588	VAL	HG13	0.931	0.017	1
1	A	588	VAL	HG21	0.931	0.017	1
1	A	588	VAL	HG22	0.931	0.017	1
1	A	588	VAL	HG23	0.931	0.017	1
1	A	588	VAL	C	176.664	0	1
1	A	588	VAL	CA	62.949	0.009	1
1	A	588	VAL	CB	32.799	0.034	1
1	A	588	VAL	CG1	21.122	0.056	1
1	A	588	VAL	CG2	21.122	0.056	1
1	A	588	VAL	N	119.01	0.061	1
1	A	589	THR	H	8.24	0.003	1
1	A	589	THR	HA	4.098	0	1
1	A	589	THR	C	178.131	0	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	589	THR	CA	63.067	0.012	1
1	A	589	THR	N	119.209	0	1
1	A	592	SER	H	8.295	0	1
1	A	592	SER	C	177.327	0	1
1	A	592	SER	CA	52.385	0	1
1	A	592	SER	N	121.424	0	1
1	A	593	ASN	H	8.373	0.002	1
1	A	593	ASN	HA	4.591	0.006	1
1	A	593	ASN	HB2	2.648	0.008	2
1	A	593	ASN	HB3	2.648	0.008	2
1	A	593	ASN	C	176.074	0	1
1	A	593	ASN	CA	54.536	0.003	1
1	A	593	ASN	CB	41.417	0	1
1	A	593	ASN	N	122.113	0	1
1	A	594	ARG	H	8.279	0	1
1	A	594	ARG	HA	4.312	0.003	1
1	A	594	ARG	HB2	1.875	0	2
1	A	594	ARG	HB3	1.778	0.002	2
1	A	594	ARG	HD2	3.186	0.002	2
1	A	594	ARG	HD3	3.186	0.002	2
1	A	594	ARG	HG2	1.628	0.003	2
1	A	594	ARG	HG3	1.628	0.003	2
1	A	594	ARG	C	177.364	0	1
1	A	594	ARG	CA	56.682	0.057	1
1	A	594	ARG	CB	30.81	0.009	1
1	A	594	ARG	CD	43.35	0.006	1
1	A	594	ARG	CG	27.338	0	1
1	A	594	ARG	N	120.374	0	1
1	A	598	SER	C	174.792	0	1
1	A	598	SER	CA	58.683	0.003	1
1	A	598	SER	CB	63.982	0	1
1	A	755	GLN	H	8.375	0.009	1
1	A	755	GLN	HA	4.289	0.074	1
1	A	755	GLN	HB2	2.073	0.017	2
1	A	755	GLN	HB3	2.073	0.017	2
1	A	755	GLN	HG2	2.403	0.008	2
1	A	755	GLN	HG3	2.403	0.008	2
1	A	755	GLN	C	176.771	0	1
1	A	755	GLN	CA	56.458	0.074	1
1	A	755	GLN	CB	29.228	0.044	1
1	A	755	GLN	CG	33.865	0.011	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	755	GLN	N	122.948	0.093	1
1	A	756	GLY	H	8.376	0.004	1
1	A	756	GLY	HA2	3.976	0.005	2
1	A	756	GLY	HA3	3.976	0.005	2
1	A	756	GLY	C	174.267	0	1
1	A	756	GLY	CA	45.482	0.026	1
1	A	756	GLY	N	109.71	0	1
1	A	757	GLN	H	8.218	0.001	1
1	A	757	GLN	HA	4.387	0.004	1
1	A	757	GLN	HB2	2.141	0.013	2
1	A	757	GLN	HB3	2.014	0.012	2
1	A	757	GLN	HG2	2.375	0.004	2
1	A	757	GLN	HG3	2.375	0.004	2
1	A	757	GLN	C	176.14	0	1
1	A	757	GLN	CA	55.88	0.047	1
1	A	757	GLN	CB	29.462	0.075	1
1	A	757	GLN	CG	33.818	0.002	1
1	A	757	GLN	N	119.803	0	1
1	A	758	SER	H	8.358	0.005	1
1	A	758	SER	HA	4.434	0.004	1
1	A	758	SER	HB2	3.878	0.009	2
1	A	758	SER	HB3	3.878	0.009	2
1	A	758	SER	C	174.068	0	1
1	A	758	SER	CA	58.428	0.018	1
1	A	758	SER	CB	63.882	0.059	1
1	A	758	SER	N	116.921	0.045	1
1	A	759	ALA	H	8.301	0.018	1
1	A	759	ALA	HA	4.338	0.004	1
1	A	759	ALA	HB1	1.382	0.015	1
1	A	759	ALA	HB2	1.382	0.015	1
1	A	759	ALA	HB3	1.382	0.015	1
1	A	759	ALA	C	177.336	0	1
1	A	759	ALA	CA	52.485	0.157	1
1	A	759	ALA	CB	19.342	0.021	1
1	A	759	ALA	N	125.764	0.009	1
1	A	760	LYS	H	8.306	0.006	1
1	A	760	LYS	HA	4.613	0.002	1
1	A	760	LYS	HB2	1.838	0	2
1	A	760	LYS	HB3	1.733	0	2
1	A	760	LYS	HD2	1.706	0.005	2
1	A	760	LYS	HD3	1.706	0.005	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	760	LYS	HE2	3.013	0.002	2
1	A	760	LYS	HE3	3.013	0.002	2
1	A	760	LYS	HG2	1.476	0.001	2
1	A	760	LYS	HG3	1.476	0.001	2
1	A	760	LYS	C	174.58	0	1
1	A	760	LYS	CA	54.149	0.03	1
1	A	760	LYS	CB	32.698	0.053	1
1	A	760	LYS	CD	29.198	0	1
1	A	760	LYS	CE	42.229	0	1
1	A	760	LYS	CG	24.469	0	1
1	A	760	LYS	N	122.17	0.005	1
1	A	761	PRO	HA	4.443	0.001	1
1	A	761	PRO	HB2	2.299	0.002	2
1	A	761	PRO	HB3	1.996	0.007	2
1	A	761	PRO	HD2	3.799	0.024	2
1	A	761	PRO	HD3	3.693	0.014	2
1	A	761	PRO	HG2	2.055	0	2
1	A	761	PRO	HG3	2.055	0	2
1	A	761	PRO	C	176.422	0	1
1	A	761	PRO	CA	63.429	0.007	1
1	A	761	PRO	CB	32.147	0.021	1
1	A	761	PRO	CD	50.697	0.016	1
1	A	761	PRO	CG	32.142	0	1
1	A	762	GLY	H	8.013	0.007	1
1	A	762	GLY	HA2	3.774	0.013	2
1	A	762	GLY	HA3	3.774	0.013	2
1	A	762	GLY	C	179.035	0	1
1	A	762	GLY	CA	46.136	0.024	1
1	A	762	GLY	N	115.579	0.041	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	175	-0.37 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	154	0.17 ± 0.24	None needed (< 0.5 ppm)
$^{13}\text{C}'$	173	-0.02 ± 0.17	None needed (< 0.5 ppm)
^{15}N	167	0.23 ± 0.42	None needed (< 0.5 ppm)

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 86%, i.e. 1676 atoms were assigned a chemical shift out of a possible 1940. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	700/709 (99%)	283/289 (98%)	280/282 (99%)	137/138 (99%)
Sidechain	873/1038 (84%)	584/672 (87%)	270/325 (83%)	19/41 (46%)
Aromatic	103/193 (53%)	70/96 (73%)	27/88 (31%)	6/9 (67%)
Overall	1676/1940 (86%)	937/1057 (89%)	577/695 (83%)	162/188 (86%)

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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	724	ARG	HD3	0.94	1.81 – 4.39	-8.4
1	A	659	HIS	CE1	121.65	126.08 – 149.12	-6.9
1	A	720	ASN	HB3	0.59	1.12 – 4.38	-6.6
1	A	625	ARG	HG2	-0.15	0.26 – 2.87	-6.6
1	A	724	ARG	HG3	-0.29	0.15 – 2.94	-6.6
1	A	625	ARG	HG3	-0.15	0.15 – 2.94	-6.1
1	A	691	ILE	HG21	-0.79	-0.56 – 2.11	-5.9
1	A	691	ILE	HG22	-0.79	-0.56 – 2.11	-5.9
1	A	691	ILE	HG23	-0.79	-0.56 – 2.11	-5.9
1	A	667	ARG	HG2	0.13	0.26 – 2.87	-5.5
1	A	745	LEU	HD11	-0.64	-0.61 – 2.12	-5.1
1	A	745	LEU	HD12	-0.64	-0.61 – 2.12	-5.1
1	A	745	LEU	HD13	-0.64	-0.61 – 2.12	-5.1
1	A	667	ARG	HG3	0.13	0.15 – 2.94	-5.1

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

