



Full wwPDB NMR Structure Validation Report ⓘ

Jan 10, 2022 – 12:24 pm GMT

PDB ID : 7BGH
Title : Solution structure of the chloroplast outer envelope channel OEP21
Authors : Hagn, F.; Haeusler, E.
Deposited on : 2021-01-07

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

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

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:

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 : 2.24
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.24

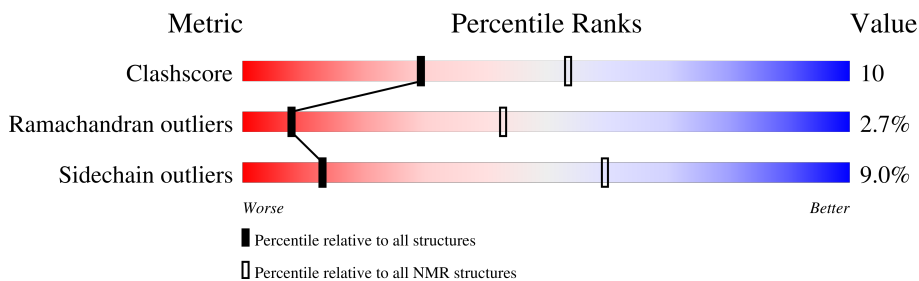
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 44%.

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	189	

2 Ensemble composition and analysis i

This entry contains 10 models. Model 10 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:1-A:8, A:13-A:37, A:45-A:54, A:59-A:69, A:81-A:92, A:101-A:129, A:138-A:145, A:152-A:177 (129)	0.39	10

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. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2863 atoms, of which 1415 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Outer envelope pore protein 21, chloroplastic.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	177	2863	921	1415	259	266	2	0

There are 12 discrepancies between the modelled and reference sequences:

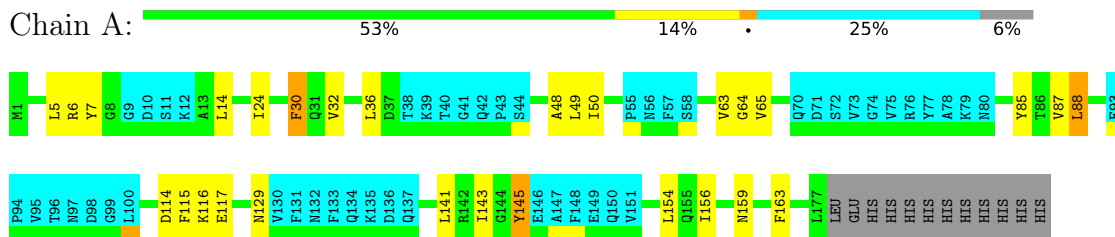
Chain	Residue	Modelled	Actual	Comment	Reference
A	178	LEU	-	expression tag	UNP Q9SM57
A	179	GLU	-	expression tag	UNP Q9SM57
A	180	HIS	-	expression tag	UNP Q9SM57
A	181	HIS	-	expression tag	UNP Q9SM57
A	182	HIS	-	expression tag	UNP Q9SM57
A	183	HIS	-	expression tag	UNP Q9SM57
A	184	HIS	-	expression tag	UNP Q9SM57
A	185	HIS	-	expression tag	UNP Q9SM57
A	186	HIS	-	expression tag	UNP Q9SM57
A	187	HIS	-	expression tag	UNP Q9SM57
A	188	HIS	-	expression tag	UNP Q9SM57
A	189	HIS	-	expression tag	UNP Q9SM57

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Outer envelope pore protein 21, chloroplastic

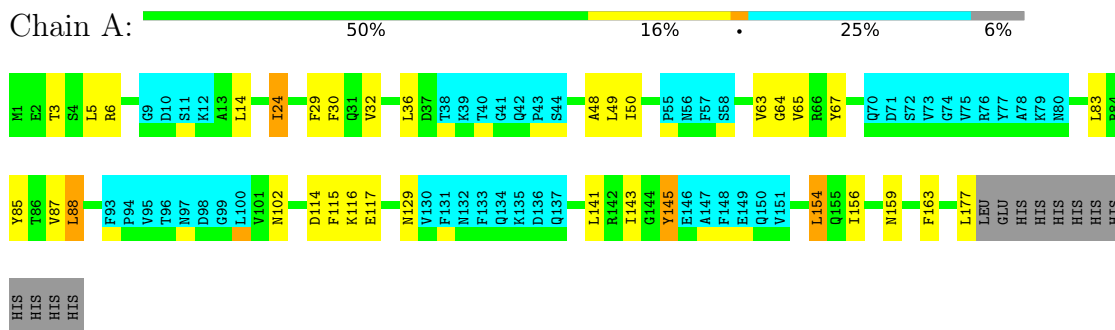


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Outer envelope pore protein 21, chloroplastic



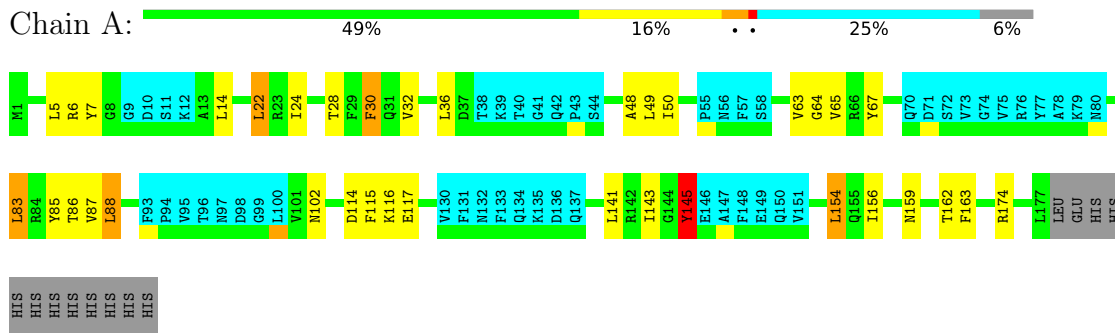
4.2.2 Score per residue for model 2

- Molecule 1: Outer envelope pore protein 21, chloroplastic

HIS
HIS
HIS
HIS

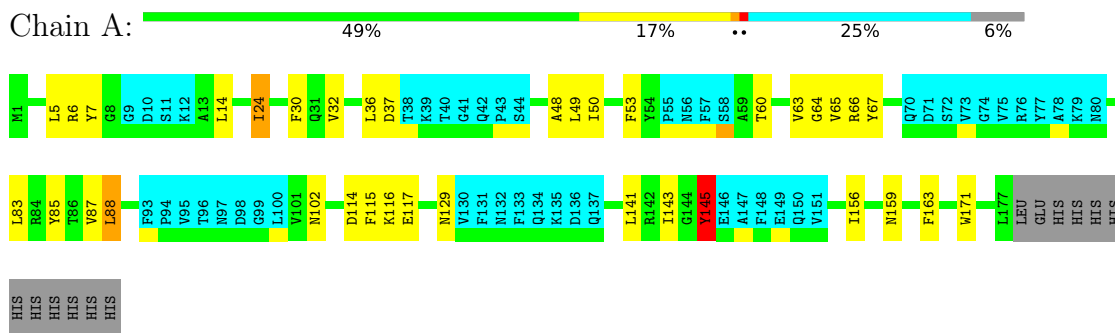
4.2.6 Score per residue for model 6

- Molecule 1: Outer envelope pore protein 21, chloroplastic



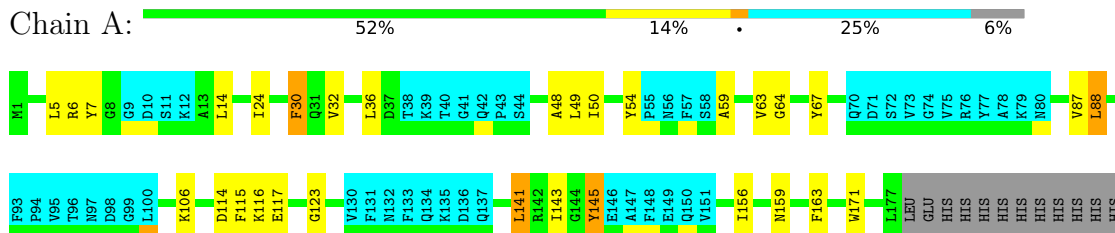
4.2.7 Score per residue for model 7

- Molecule 1: Outer envelope pore protein 21, chloroplastic



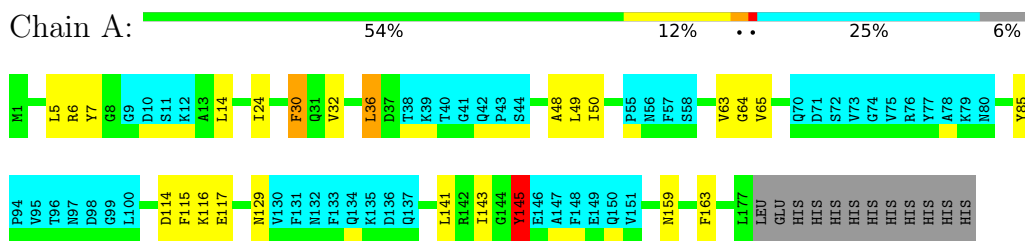
4.2.8 Score per residue for model 8

- Molecule 1: Outer envelope pore protein 21, chloroplastic



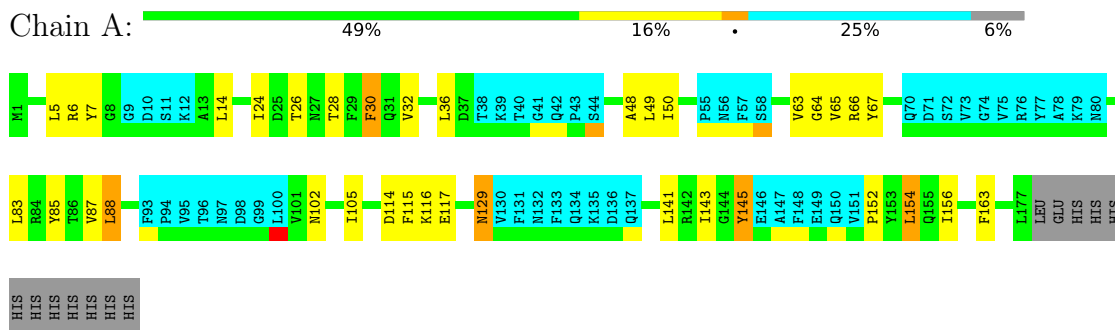
4.2.9 Score per residue for model 9

- Molecule 1: Outer envelope pore protein 21, chloroplastic



4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Outer envelope pore protein 21, chloroplastic



5 Refinement protocol and experimental data overview

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

Of the 50 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	structure calculation	
X-PLOR NIH	refinement	

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	980
Number of shifts mapped to atoms	980
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	44%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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	0.65±0.00	0±0/1097 (0.0± 0.0%)	0.97±0.01	0±0/1474 (0.0± 0.0%)
All	All	0.65	0/10970 (0.0%)	0.97	5/14740 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
All	All	0	1

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	145	TYR	CB-CG-CD2	-5.90	117.46	121.00	6	5

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	142	ARG	Peptide	1

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	1072	1064	1064	22±3
All	All	10720	10640	10640	218

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:LEU:HD21	1:A:14:LEU:HD22	0.77	1.57	4	9
1:A:115:PHE:O	1:A:117:GLU:N	0.72	2.23	9	10
1:A:5:LEU:HD21	1:A:14:LEU:HD21	0.63	1.69	2	1
1:A:5:LEU:HD23	1:A:6:ARG:N	0.62	2.09	2	10
1:A:141:LEU:HB3	1:A:156:ILE:HG22	0.60	1.73	4	1
1:A:141:LEU:HD22	1:A:141:LEU:O	0.59	1.96	4	1
1:A:105:ILE:HG22	1:A:124:ALA:HB1	0.59	1.74	2	2
1:A:67:TYR:CD1	1:A:83:LEU:HD23	0.58	2.33	10	3
1:A:65:VAL:HG12	1:A:85:TYR:CB	0.58	2.28	5	8
1:A:14:LEU:HD13	1:A:15:LYS:N	0.57	2.15	2	1
1:A:54:TYR:CZ	1:A:59:ALA:HB3	0.56	2.35	8	1
1:A:49:LEU:C	1:A:50:ILE:HD13	0.56	2.21	7	6
1:A:143:ILE:H	1:A:143:ILE:HD12	0.56	1.59	4	2
1:A:86:THR:HG23	1:A:109:CYS:O	0.54	2.02	2	1
1:A:28:THR:HG22	1:A:52:HIS:CE1	0.53	2.39	5	1
1:A:143:ILE:HG22	1:A:145:TYR:HB3	0.52	1.80	3	7
1:A:154:LEU:HD23	1:A:154:LEU:N	0.51	2.20	5	4
1:A:5:LEU:HD21	1:A:14:LEU:CD2	0.51	2.34	2	2
1:A:49:LEU:HD23	1:A:64:GLY:HA2	0.51	1.83	6	9
1:A:24:ILE:HD11	1:A:30:PHE:HB2	0.51	1.82	5	8
1:A:106:LYS:N	1:A:123:GLY:O	0.50	2.43	4	2
1:A:86:THR:HG23	1:A:109:CYS:C	0.50	2.27	2	1
1:A:111:VAL:HG23	1:A:118:TRP:CD1	0.49	2.42	2	2
1:A:49:LEU:HD23	1:A:64:GLY:CA	0.49	2.38	10	9
1:A:36:LEU:HD23	1:A:37:ASP:O	0.49	2.06	7	1
1:A:87:VAL:C	1:A:88:LEU:HD13	0.48	2.28	2	10
1:A:49:LEU:HD13	1:A:50:ILE:N	0.48	2.23	2	1
1:A:67:TYR:CE1	1:A:83:LEU:HD11	0.48	2.42	6	1
1:A:24:ILE:HD13	1:A:28:THR:HG22	0.48	1.85	6	3
1:A:88:LEU:N	1:A:88:LEU:HD13	0.47	2.24	4	6
1:A:36:LEU:C	1:A:36:LEU:HD22	0.47	2.30	3	1
1:A:141:LEU:HD22	1:A:141:LEU:C	0.46	2.29	4	1
1:A:88:LEU:HD13	1:A:88:LEU:N	0.46	2.26	2	4
1:A:32:VAL:HG12	1:A:48:ALA:CB	0.46	2.41	10	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:HD22	1:A:36:LEU:C	0.46	2.31	9	1
1:A:5:LEU:CG	1:A:14:LEU:HD11	0.46	2.41	2	1
1:A:111:VAL:HG23	1:A:118:TRP:HD1	0.46	1.71	3	1
1:A:66:ARG:O	1:A:83:LEU:HD22	0.46	2.10	10	2
1:A:177:LEU:H	1:A:177:LEU:HD23	0.45	1.70	5	2
1:A:24:ILE:HD11	1:A:30:PHE:N	0.45	2.26	10	1
1:A:105:ILE:HG22	1:A:124:ALA:CB	0.45	2.39	2	2
1:A:88:LEU:HD12	1:A:121:ARG:NH2	0.45	2.27	3	1
1:A:143:ILE:HD12	1:A:143:ILE:N	0.45	2.26	10	9
1:A:162:THR:HG21	1:A:174:ARG:NH2	0.45	2.27	6	1
1:A:156:ILE:HD11	1:A:163:PHE:CD1	0.44	2.47	5	1
1:A:67:TYR:CE1	1:A:83:LEU:HD23	0.44	2.48	10	3
1:A:65:VAL:HG12	1:A:85:TYR:HB2	0.44	1.89	6	1
1:A:36:LEU:C	1:A:36:LEU:HD23	0.44	2.33	2	6
1:A:24:ILE:N	1:A:24:ILE:HD13	0.43	2.28	1	2
1:A:53:PHE:CB	1:A:60:THR:HG22	0.43	2.44	7	1
1:A:83:LEU:HD13	1:A:83:LEU:C	0.43	2.34	7	3
1:A:50:ILE:HD13	1:A:50:ILE:N	0.42	2.29	1	5
1:A:141:LEU:O	1:A:141:LEU:HD23	0.42	2.14	8	1
1:A:156:ILE:C	1:A:156:ILE:HD12	0.42	2.35	4	6
1:A:141:LEU:H	1:A:141:LEU:HD13	0.42	1.74	4	1
1:A:24:ILE:HD11	1:A:29:PHE:C	0.42	2.35	1	1
1:A:141:LEU:HD23	1:A:141:LEU:C	0.42	2.34	8	1
1:A:5:LEU:HD23	1:A:5:LEU:C	0.42	2.35	9	9
1:A:65:VAL:HG12	1:A:85:TYR:HB3	0.42	1.92	7	2
1:A:143:ILE:HD13	1:A:143:ILE:N	0.41	2.30	2	1
1:A:26:THR:O	1:A:26:THR:HG23	0.41	2.15	10	1
1:A:3:THR:CG2	1:A:177:LEU:HD12	0.41	2.45	1	1
1:A:156:ILE:HD12	1:A:156:ILE:C	0.41	2.36	3	3
1:A:5:LEU:HG	1:A:14:LEU:HD11	0.41	1.92	2	1
1:A:49:LEU:HD12	1:A:51:ARG:CG	0.41	2.46	2	1
1:A:141:LEU:CB	1:A:156:ILE:HG22	0.41	2.46	4	1
1:A:143:ILE:HD12	1:A:143:ILE:H	0.41	1.74	5	1
1:A:156:ILE:HD11	1:A:163:PHE:HD1	0.41	1.76	5	1
1:A:36:LEU:HD23	1:A:36:LEU:C	0.40	2.36	1	1
1:A:22:LEU:N	1:A:22:LEU:HD13	0.40	2.31	6	1
1:A:7:TYR:HA	1:A:14:LEU:HD23	0.40	1.93	4	1
1:A:86:THR:HG23	1:A:88:LEU:CD1	0.40	2.46	6	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	127/189 (67%)	117±2 (92±1%)	7±2 (5±1%)	3±1 (3±1%)	8	43
All	All	1270/1890 (67%)	1169 (92%)	67 (5%)	34 (3%)	8	43

All 7 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	114	ASP	10
1	A	116	LYS	10
1	A	159	ASN	9
1	A	81	ASP	2
1	A	101	VAL	1
1	A	138	ASP	1
1	A	152	PRO	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	110/164 (67%)	100±1 (91±1%)	10±1 (9±1%)	13	60
All	All	1100/1640 (67%)	1001 (91%)	99 (9%)	13	60

All 22 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	30	PHE	10
1	A	63	VAL	10
1	A	88	LEU	10

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Mol	Chain	Res	Type	Models (Total)
1	A	141	LEU	10
1	A	145	TYR	10
1	A	163	PHE	10
1	A	7	TYR	9
1	A	129	ASN	7
1	A	102	ASN	4
1	A	154	LEU	4
1	A	24	ILE	2
1	A	143	ILE	2
1	A	36	LEU	2
1	A	14	LEU	1
1	A	49	LEU	1
1	A	162	THR	1
1	A	177	LEU	1
1	A	22	LEU	1
1	A	83	LEU	1
1	A	171	TRP	1
1	A	67	TYR	1
1	A	105	ILE	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 monosaccharides 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

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 44% for the well-defined parts and 40% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: oep21-31.bmrB

7.1.1 Bookkeeping [i](#)

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	980
Number of shifts mapped to atoms	980
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 [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	155	0.46 \pm 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	132	-0.09 \pm 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	141	0.84 \pm 0.12	Should be applied
^{15}N	147	-0.30 \pm 0.34	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 44%, i.e. 745 atoms were assigned a chemical shift out of a possible 1699. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	488/643 (76%)	124/257 (48%)	242/258 (94%)	122/128 (95%)
Sidechain	193/867 (22%)	62/509 (12%)	131/300 (44%)	0/58 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	64/189 (34%)	60/99 (61%)	0/84 (0%)	4/6 (67%)
Overall	745/1699 (44%)	246/865 (28%)	373/642 (58%)	126/192 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 40%, i.e. 900 atoms were assigned a chemical shift out of a possible 2276. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	592/877 (68%)	149/350 (43%)	296/354 (84%)	147/173 (85%)
Sidechain	237/1157 (20%)	74/680 (11%)	163/403 (40%)	0/74 (0%)
Aromatic	71/242 (29%)	67/128 (52%)	0/108 (0%)	4/6 (67%)
Overall	900/2276 (40%)	290/1158 (25%)	459/865 (53%)	151/253 (60%)

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:

