



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 03:14 PM UTC

PDB ID : 2N5E / pdb_00002n5e
BMRB ID : 25710
Title : The 3D solution structure of discoidal high-density lipoprotein particles
Authors : Bibow, S.; Polyhach, Y.; Eichmann, C.; Chi, C.N.; Kowal, J.; Stahlberg, H.; Jeschke, G.; Guentert, P.; Riek, R.
Deposited on : 2015-07-15

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 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
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

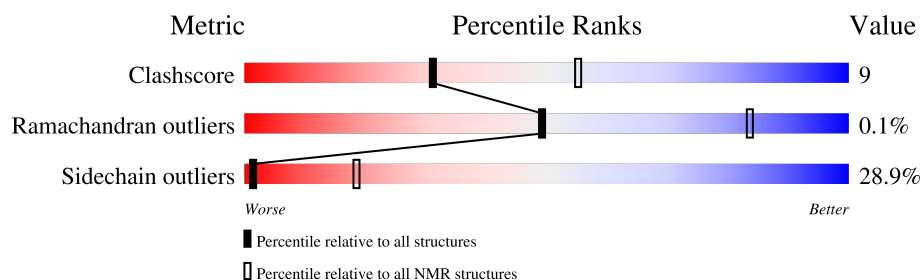
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 15%.

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	167	
1	B	167	

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:74-A:120, A:143-A:241, B:74-B:120, B:143-B:241 (292)	1.31	1

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5464 atoms, of which 2728 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						Trace
1	A	167	Total	C	H	N	O	S	0
			2732	858	1364	241	266	3	
1	B	167	Total	C	H	N	O	S	0
			2732	858	1364	241	266	3	

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP P02647
A	?	-	LEU	deletion	UNP P02647
A	?	-	ARG	deletion	UNP P02647
A	?	-	ALA	deletion	UNP P02647
A	?	-	GLU	deletion	UNP P02647
A	?	-	LEU	deletion	UNP P02647
A	?	-	GLN	deletion	UNP P02647
A	?	-	GLU	deletion	UNP P02647
A	?	-	GLY	deletion	UNP P02647
A	?	-	ALA	deletion	UNP P02647
A	?	-	ARG	deletion	UNP P02647
A	?	-	GLN	deletion	UNP P02647
A	?	-	LYS	deletion	UNP P02647
A	?	-	LEU	deletion	UNP P02647
A	?	-	HIS	deletion	UNP P02647
A	?	-	GLU	deletion	UNP P02647
A	?	-	LEU	deletion	UNP P02647
A	?	-	GLN	deletion	UNP P02647
A	?	-	GLU	deletion	UNP P02647
A	?	-	LYS	deletion	UNP P02647
A	?	-	LEU	deletion	UNP P02647
A	?	-	SER	deletion	UNP P02647
B	?	-	PRO	deletion	UNP P02647
B	?	-	LEU	deletion	UNP P02647
B	?	-	ARG	deletion	UNP P02647
B	?	-	ALA	deletion	UNP P02647
B	?	-	GLU	deletion	UNP P02647
B	?	-	LEU	deletion	UNP P02647
B	?	-	GLN	deletion	UNP P02647

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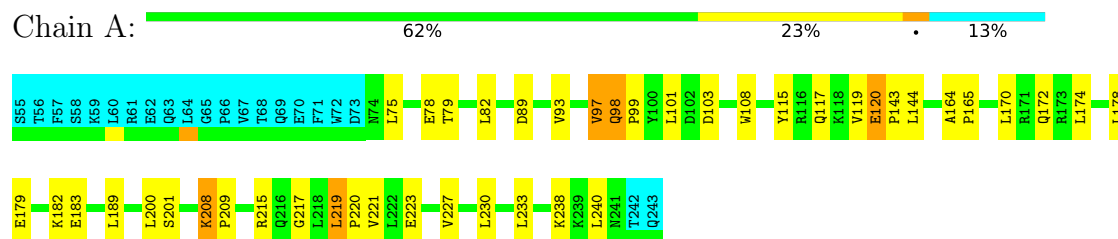
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	deletion	UNP P02647
B	?	-	GLY	deletion	UNP P02647
B	?	-	ALA	deletion	UNP P02647
B	?	-	ARG	deletion	UNP P02647
B	?	-	GLN	deletion	UNP P02647
B	?	-	LYS	deletion	UNP P02647
B	?	-	LEU	deletion	UNP P02647
B	?	-	HIS	deletion	UNP P02647
B	?	-	GLU	deletion	UNP P02647
B	?	-	LEU	deletion	UNP P02647
B	?	-	GLN	deletion	UNP P02647
B	?	-	GLU	deletion	UNP P02647
B	?	-	LYS	deletion	UNP P02647
B	?	-	LEU	deletion	UNP P02647
B	?	-	SER	deletion	UNP P02647

4 Residue-property plots

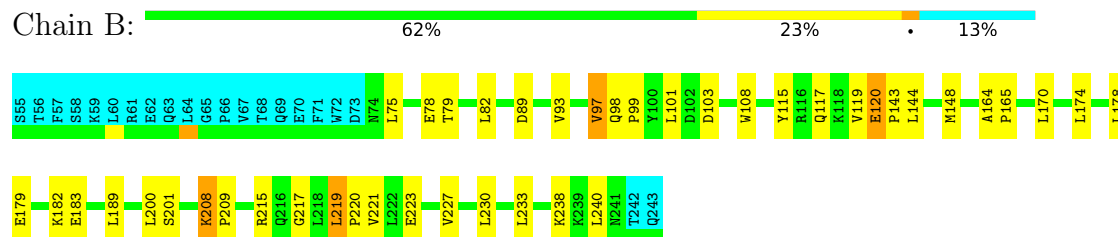
4.1 Average score per residue in the NMR ensemble

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: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I

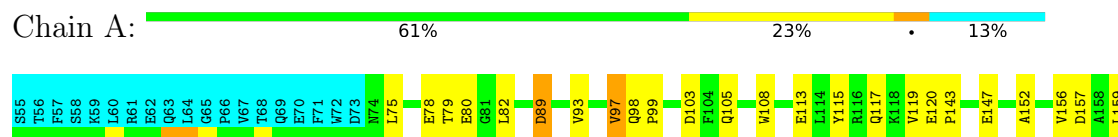


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

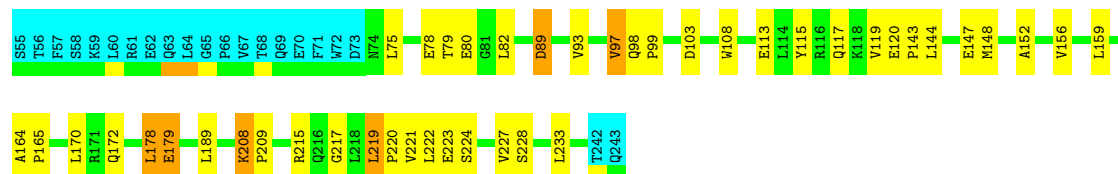
- Molecule 1: Apolipoprotein A-I





• Molecule 1: Apolipoprotein A-I

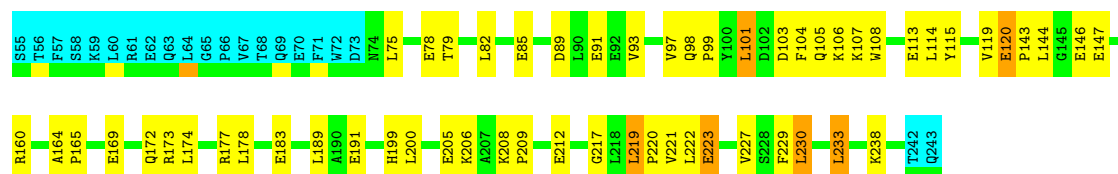
Chain B: 61% 23% • 13%



4.2.2 Score per residue for model 2

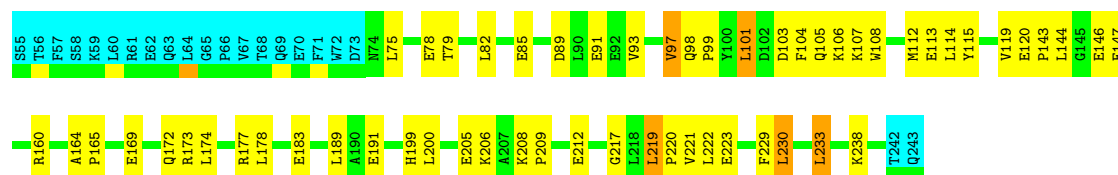
• Molecule 1: Apolipoprotein A-I

Chain A: 53% 31% • 13%



• Molecule 1: Apolipoprotein A-I

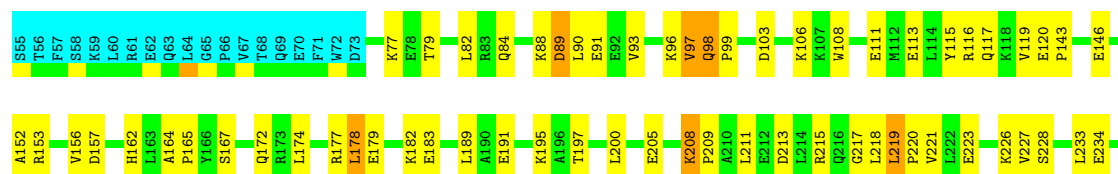
Chain B: 53% 31% • 13%

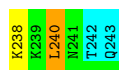


4.2.3 Score per residue for model 3

• Molecule 1: Apolipoprotein A-I

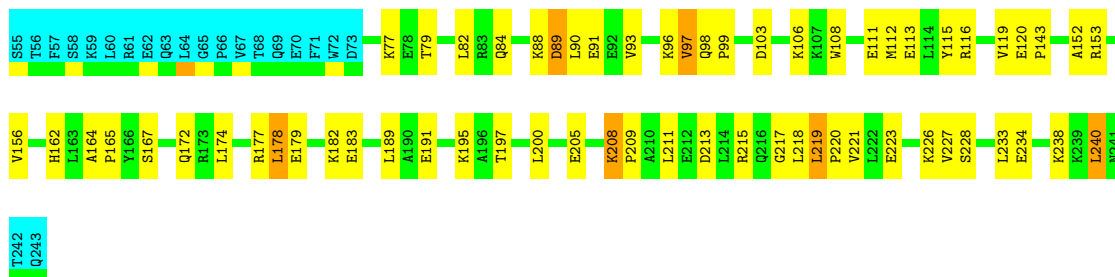
Chain A: 49% 34% • 13%





• Molecule 1: Apolipoprotein A-I

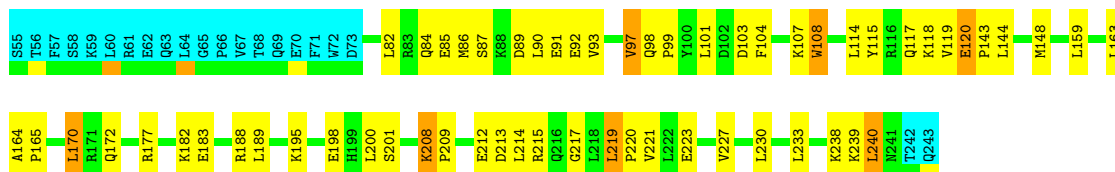
Chain B:



4.2.4 Score per residue for model 4

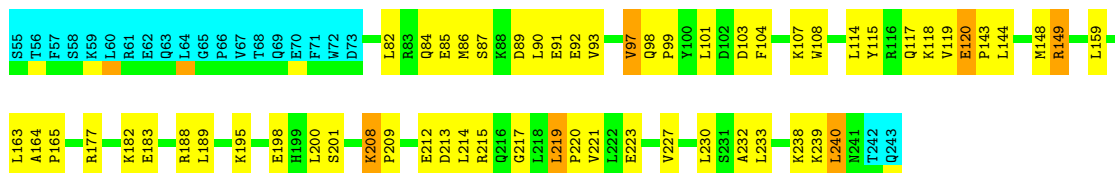
• Molecule 1: Apolipoprotein A-I

Chain A:



• Molecule 1: Apolipoprotein A-I

Chain B:

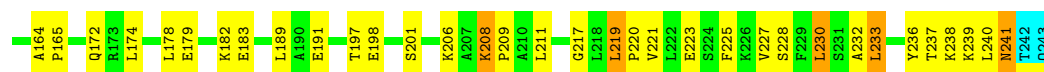


4.2.5 Score per residue for model 5

• Molecule 1: Apolipoprotein A-I

Chain A:



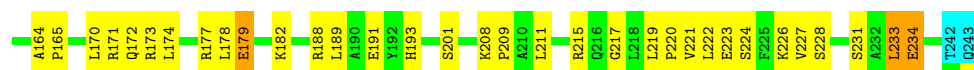
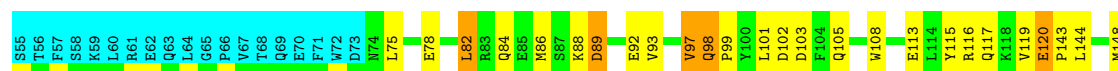


• Molecule 1: Apolipoprotein A-I

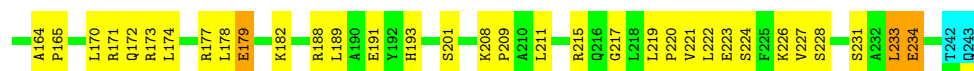
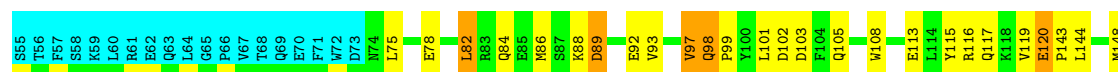


4.2.6 Score per residue for model 6

• Molecule 1: Apolipoprotein A-I



• Molecule 1: Apolipoprotein A-I

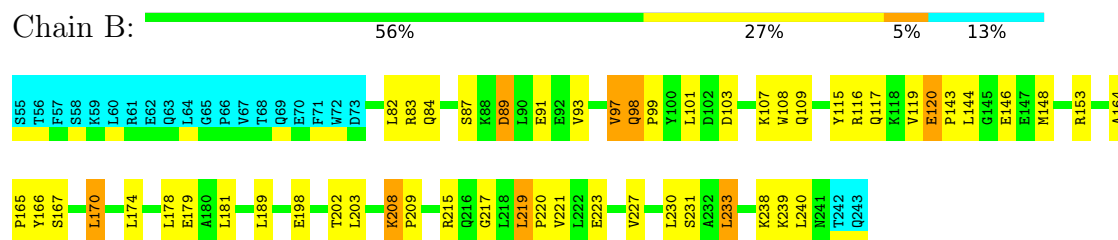


4.2.7 Score per residue for model 7

• Molecule 1: Apolipoprotein A-I

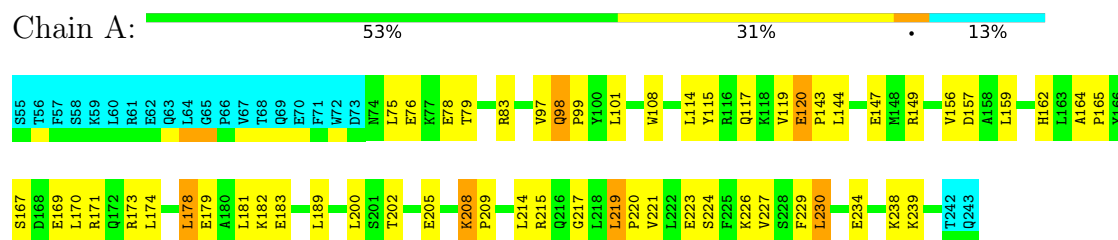


• Molecule 1: Apolipoprotein A-I

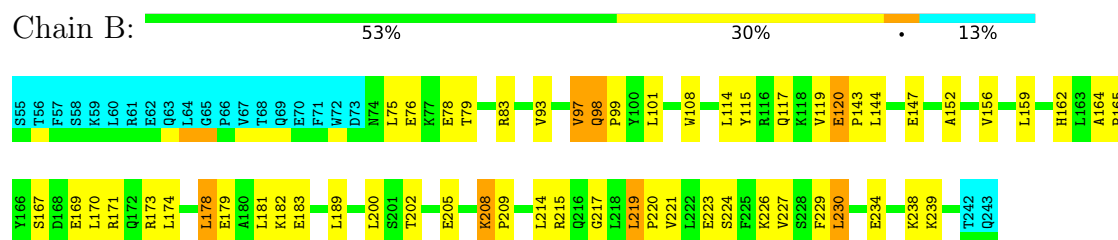


4.2.8 Score per residue for model 8

- Molecule 1: Apolipoprotein A-I

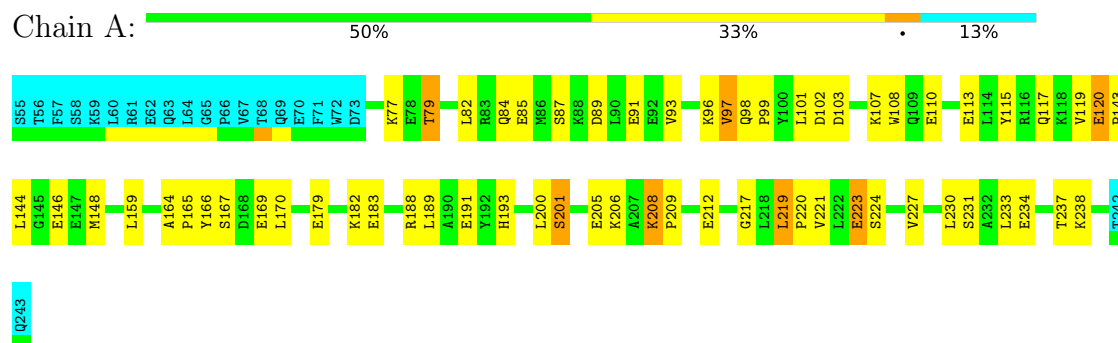


- Molecule 1: Apolipoprotein A-I



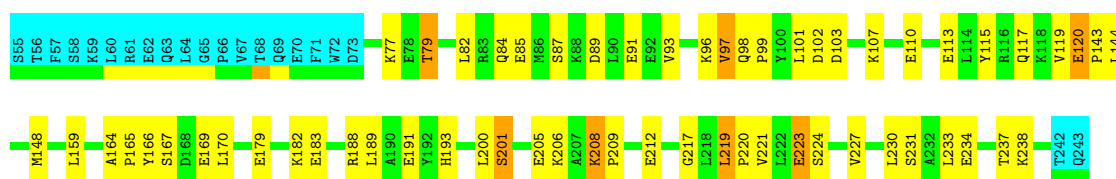
4.2.9 Score per residue for model 9

- Molecule 1: Apolipoprotein A-I



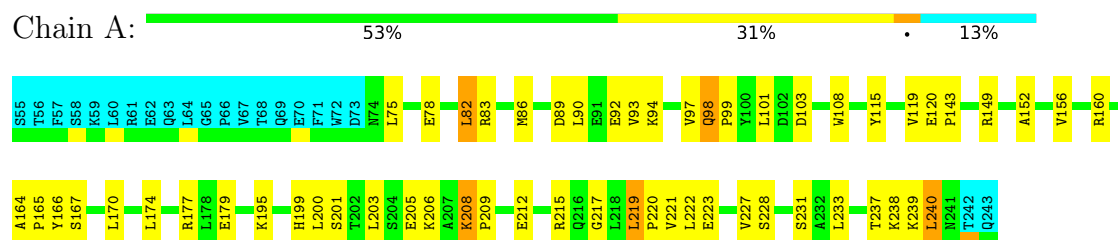
- Molecule 1: Apolipoprotein A-I



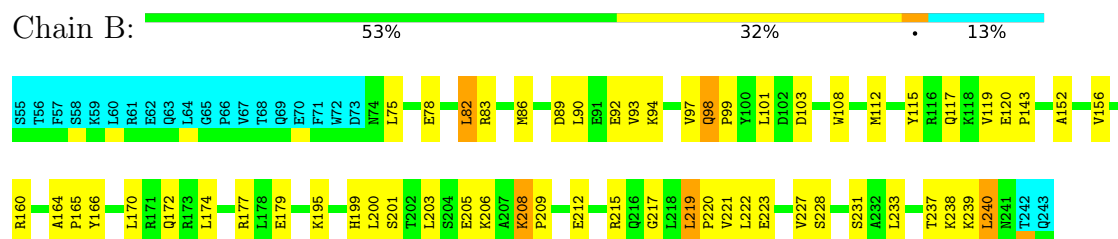


4.2.10 Score per residue for model 10

- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	3.97
CYANA	refinement	3.97

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	689
Number of shifts mapped to atoms	689
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	15%

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	1192	1198	1198	22±2
1	B	1192	1198	1198	22±2
All	All	23840	23960	23960	419

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:THR:HG22	1:A:82:LEU:HD23	0.81	1.52	3	2
1:B:79:THR:HG22	1:B:82:LEU:HD23	0.79	1.53	3	2
1:A:197:THR:HG23	1:B:240:LEU:HD13	0.79	1.54	5	1
1:A:240:LEU:HD13	1:B:197:THR:HG23	0.76	1.56	5	1
1:B:164:ALA:HB3	1:B:165:PRO:HD3	0.69	1.64	7	10
1:A:164:ALA:HB3	1:A:165:PRO:HD3	0.69	1.64	7	10
1:A:115:TYR:O	1:A:119:VAL:HG23	0.68	1.88	5	10
1:A:75:LEU:O	1:A:79:THR:HG23	0.67	1.90	5	2
1:B:75:LEU:O	1:B:79:THR:HG23	0.67	1.90	5	2
1:B:115:TYR:O	1:B:119:VAL:HG23	0.66	1.91	1	10
1:B:230:LEU:HD22	1:B:233:LEU:HD11	0.66	1.68	7	1
1:A:164:ALA:HB3	1:A:165:PRO:CD	0.64	2.23	7	10
1:B:164:ALA:HB3	1:B:165:PRO:CD	0.64	2.23	3	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:230:LEU:HD22	1:A:233:LEU:HD11	0.64	1.68	7	1
1:B:223:GLU:O	1:B:227:VAL:HG23	0.64	1.93	6	8
1:A:223:GLU:O	1:A:227:VAL:HG23	0.63	1.93	6	9
1:A:201:SER:OG	1:B:237:THR:HG23	0.62	1.94	9	1
1:A:89:ASP:O	1:A:93:VAL:HG23	0.61	1.96	4	9
1:B:89:ASP:O	1:B:93:VAL:HG23	0.61	1.95	4	9
1:B:233:LEU:O	1:B:237:THR:HG23	0.60	1.96	5	1
1:A:230:LEU:HD13	1:A:233:LEU:HD11	0.60	1.73	5	2
1:A:233:LEU:O	1:A:237:THR:HG23	0.60	1.96	5	1
1:A:230:LEU:CD2	1:A:233:LEU:HD11	0.60	2.27	7	1
1:B:98:GLN:CB	1:B:99:PRO:CD	0.59	2.80	8	10
1:B:230:LEU:CD2	1:B:233:LEU:HD11	0.59	2.27	7	1
1:A:233:LEU:HD23	1:A:234:GLU:N	0.59	2.12	6	1
1:A:237:THR:HG23	1:B:201:SER:OG	0.59	1.97	9	1
1:A:236:TYR:CZ	1:A:240:LEU:HD11	0.59	2.31	5	1
1:B:236:TYR:CZ	1:B:240:LEU:HD11	0.59	2.31	5	1
1:B:230:LEU:HD13	1:B:233:LEU:HD11	0.59	1.73	5	2
1:B:233:LEU:HD23	1:B:234:GLU:N	0.58	2.12	6	1
1:B:82:LEU:HD13	1:B:82:LEU:O	0.58	1.99	5	3
1:A:82:LEU:O	1:A:82:LEU:HD13	0.58	1.99	5	3
1:B:152:ALA:O	1:B:156:VAL:HG12	0.57	1.98	3	4
1:A:166:TYR:CZ	1:A:170:LEU:HD23	0.56	2.36	7	1
1:A:98:GLN:CB	1:A:99:PRO:CD	0.56	2.84	8	10
1:A:120:GLU:CB	1:A:143:PRO:CD	0.55	2.84	6	10
1:B:166:TYR:CZ	1:B:170:LEU:HD23	0.55	2.35	7	1
1:B:120:GLU:CB	1:B:143:PRO:CD	0.55	2.84	7	10
1:A:197:THR:CG2	1:B:240:LEU:HD13	0.55	2.32	5	1
1:A:215:ARG:O	1:A:219:LEU:HD13	0.54	2.01	8	1
1:B:215:ARG:O	1:B:219:LEU:HD13	0.54	2.01	8	1
1:B:223:GLU:O	1:B:227:VAL:HG13	0.54	2.03	10	1
1:A:82:LEU:HD23	1:A:83:ARG:N	0.53	2.18	10	1
1:B:82:LEU:HD23	1:B:83:ARG:N	0.53	2.19	10	1
1:A:223:GLU:O	1:A:227:VAL:HG13	0.53	2.03	10	1
1:A:170:LEU:C	1:A:170:LEU:HD13	0.52	2.29	4	3
1:A:208:LYS:CB	1:A:209:PRO:CD	0.52	2.87	8	10
1:B:208:LYS:CB	1:B:209:PRO:CD	0.52	2.87	8	10
1:A:152:ALA:O	1:A:156:VAL:HG12	0.52	2.04	10	3
1:A:219:LEU:CB	1:A:220:PRO:CD	0.52	2.88	8	10
1:B:219:LEU:CB	1:B:220:PRO:CD	0.51	2.88	8	10
1:A:240:LEU:HD13	1:B:197:THR:CG2	0.51	2.34	5	1
1:A:114:LEU:HD13	1:A:114:LEU:O	0.51	2.06	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:217:GLY:O	1:A:221:VAL:HG23	0.50	2.07	2	10
1:A:178:LEU:HD23	1:A:179:GLU:N	0.50	2.21	8	2
1:B:236:TYR:CE2	1:B:240:LEU:HD11	0.50	2.41	5	1
1:B:114:LEU:O	1:B:114:LEU:HD13	0.50	2.06	8	1
1:B:178:LEU:HD23	1:B:179:GLU:N	0.50	2.21	8	2
1:A:236:TYR:CE2	1:A:240:LEU:HD11	0.49	2.41	5	1
1:B:217:GLY:O	1:B:221:VAL:HG23	0.49	2.07	2	10
1:A:164:ALA:CB	1:A:165:PRO:CD	0.48	2.91	3	10
1:A:178:LEU:HD12	1:A:179:GLU:N	0.48	2.24	7	3
1:B:170:LEU:C	1:B:170:LEU:HD13	0.48	2.33	1	2
1:B:164:ALA:CB	1:B:165:PRO:CD	0.48	2.91	1	9
1:A:237:THR:HG23	1:B:201:SER:HB3	0.48	1.83	10	1
1:A:93:VAL:O	1:A:97:VAL:HG23	0.47	2.09	9	7
1:B:98:GLN:CB	1:B:99:PRO:HD3	0.47	2.38	8	10
1:A:240:LEU:O	1:A:240:LEU:HD13	0.47	2.09	4	1
1:B:93:VAL:O	1:B:97:VAL:HG23	0.47	2.09	4	9
1:A:211:LEU:C	1:A:211:LEU:HD13	0.47	2.35	5	2
1:B:230:LEU:C	1:B:230:LEU:HD13	0.47	2.35	7	1
1:A:230:LEU:C	1:A:230:LEU:HD13	0.47	2.35	7	1
1:B:178:LEU:HD12	1:B:179:GLU:N	0.47	2.24	7	3
1:B:159:LEU:O	1:B:163:LEU:HD23	0.47	2.10	4	1
1:B:166:TYR:CE2	1:B:170:LEU:HD22	0.47	2.44	10	1
1:A:159:LEU:O	1:A:163:LEU:HD23	0.47	2.10	4	1
1:B:240:LEU:O	1:B:240:LEU:HD13	0.47	2.09	4	1
1:A:197:THR:HG21	1:B:240:LEU:HD22	0.46	1.87	3	1
1:B:211:LEU:HD13	1:B:211:LEU:C	0.46	2.35	3	2
1:A:114:LEU:HD13	1:A:114:LEU:C	0.46	2.35	8	1
1:B:114:LEU:HD13	1:B:114:LEU:C	0.46	2.35	8	1
1:B:144:LEU:HD12	1:B:148:MET:HE3	0.46	1.87	1	1
1:B:166:TYR:CZ	1:B:170:LEU:HD22	0.46	2.45	10	1
1:A:230:LEU:O	1:A:230:LEU:HD13	0.46	2.11	8	1
1:A:166:TYR:CZ	1:A:170:LEU:HD22	0.46	2.45	10	1
1:A:201:SER:HB3	1:B:237:THR:HG23	0.45	1.87	10	1
1:B:117:GLN:O	1:B:143:PRO:CD	0.45	2.64	6	6
1:A:117:GLN:O	1:A:143:PRO:CD	0.45	2.65	1	6
1:B:230:LEU:O	1:B:230:LEU:HD13	0.45	2.11	8	1
1:A:166:TYR:CE2	1:A:170:LEU:HD22	0.45	2.46	10	1
1:A:79:THR:HG23	1:A:82:LEU:HD23	0.45	1.88	9	1
1:B:79:THR:HG23	1:B:82:LEU:HD23	0.44	1.88	9	1
1:A:98:GLN:CB	1:A:99:PRO:HD3	0.44	2.42	8	10
1:B:219:LEU:N	1:B:220:PRO:HD2	0.44	2.28	5	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:LEU:HD23	1:B:160:ARG:HB3	0.44	1.89	2	1
1:B:120:GLU:CB	1:B:143:PRO:HD3	0.43	2.43	6	9
1:A:120:GLU:CB	1:A:143:PRO:HD3	0.43	2.43	6	8
1:A:240:LEU:HD22	1:B:197:THR:HG21	0.43	1.88	3	1
1:B:208:LYS:N	1:B:209:PRO:HD2	0.43	2.28	2	2
1:A:219:LEU:N	1:A:220:PRO:HD2	0.43	2.28	5	7
1:B:166:TYR:O	1:B:170:LEU:HD13	0.43	2.14	9	1
1:A:166:TYR:O	1:A:170:LEU:HD13	0.43	2.14	9	1
1:A:79:THR:O	1:A:82:LEU:HD23	0.43	2.14	2	2
1:A:208:LYS:N	1:A:209:PRO:HD2	0.42	2.28	2	2
1:B:79:THR:O	1:B:82:LEU:HD23	0.42	2.14	2	2
1:A:170:LEU:HD22	1:A:170:LEU:O	0.42	2.14	4	1
1:B:97:VAL:O	1:B:98:GLN:C	0.42	2.62	4	2
1:A:156:VAL:CG1	1:A:157:ASP:N	0.42	2.83	8	1
1:A:197:THR:HG21	1:B:240:LEU:HD13	0.41	1.92	7	1
1:B:120:GLU:N	1:B:143:PRO:HD2	0.41	2.30	1	1
1:A:208:LYS:CB	1:A:209:PRO:HD3	0.41	2.46	8	1
1:A:120:GLU:N	1:A:143:PRO:HD2	0.41	2.31	5	2
1:A:160:ARG:HB3	1:B:101:LEU:HD23	0.41	1.92	2	1
1:B:82:LEU:HD23	1:B:83:ARG:H	0.41	1.75	7	1
1:A:156:VAL:HG13	1:A:157:ASP:N	0.41	2.31	1	2
1:B:170:LEU:HD22	1:B:170:LEU:O	0.41	2.16	1	1
1:B:208:LYS:CB	1:B:209:PRO:HD3	0.41	2.46	8	2
1:A:189:LEU:C	1:A:189:LEU:HD12	0.40	2.41	6	1
1:B:189:LEU:C	1:B:189:LEU:HD12	0.40	2.41	6	1
1:A:108:TRP:HE1	1:B:149:ARG:NH1	0.40	2.14	4	1
1:A:82:LEU:HD23	1:A:83:ARG:H	0.40	1.75	7	1
1:A:219:LEU:CB	1:A:220:PRO:HD3	0.40	2.47	8	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	146/167 (87%)	141±1 (97±1%)	5±1 (3±1%)	0±0 (0±0%)	49	83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	146/167 (87%)	141±1 (97±1%)	5±1 (3±1%)	0±0 (0±0%)	49 83
All	All	2920/3340 (87%)	2824 (97%)	94 (3%)	2 (0%)	49 83

All 2 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	241	ASN	1
1	B	241	ASN	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	126/146 (86%)	89±6 (71±5%)	37±6 (29±5%)	1 18
1	B	126/146 (86%)	90±6 (71±5%)	36±6 (29±5%)	1 19
All	All	2520/2920 (86%)	1791 (71%)	729 (29%)	1 18

All 195 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	97	VAL	10
1	A	108	TRP	10
1	B	97	VAL	10
1	A	219	LEU	9
1	A	233	LEU	9
1	B	108	TRP	9
1	B	219	LEU	9
1	B	233	LEU	9
1	A	103	ASP	8
1	A	189	LEU	8
1	A	208	LYS	8
1	B	103	ASP	8
1	B	189	LEU	8
1	B	208	LYS	8

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Mol	Chain	Res	Type	Models (Total)
1	A	101	LEU	8
1	A	238	LYS	8
1	B	101	LEU	8
1	B	238	LYS	8
1	A	144	LEU	7
1	A	174	LEU	7
1	B	144	LEU	7
1	B	174	LEU	7
1	A	78	GLU	6
1	A	172	GLN	6
1	A	215	ARG	6
1	B	78	GLU	6
1	B	215	ARG	6
1	A	183	GLU	6
1	A	200	LEU	6
1	B	183	GLU	6
1	B	200	LEU	6
1	A	182	LYS	6
1	B	182	LYS	6
1	A	113	GLU	5
1	A	178	LEU	5
1	A	179	GLU	5
1	A	228	SER	5
1	B	113	GLU	5
1	B	172	GLN	5
1	B	178	LEU	5
1	B	179	GLU	5
1	B	228	SER	5
1	A	91	GLU	5
1	A	120	GLU	5
1	A	177	ARG	5
1	A	191	GLU	5
1	A	205	GLU	5
1	A	230	LEU	5
1	B	91	GLU	5
1	B	177	ARG	5
1	B	191	GLU	5
1	B	205	GLU	5
1	B	230	LEU	5
1	A	84	GLN	5
1	A	98	GLN	5
1	A	167	SER	5

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Mol	Chain	Res	Type	Models (Total)
1	B	84	GLN	5
1	A	148	MET	5
1	A	239	LYS	5
1	B	120	GLU	5
1	B	148	MET	5
1	B	239	LYS	5
1	A	75	LEU	4
1	A	89	ASP	4
1	A	105	GLN	4
1	A	147	GLU	4
1	A	159	LEU	4
1	A	222	LEU	4
1	A	224	SER	4
1	B	75	LEU	4
1	B	89	ASP	4
1	B	147	GLU	4
1	B	159	LEU	4
1	B	222	LEU	4
1	B	224	SER	4
1	A	85	GLU	4
1	A	107	LYS	4
1	A	146	GLU	4
1	A	206	LYS	4
1	A	212	GLU	4
1	B	85	GLU	4
1	B	107	LYS	4
1	B	206	LYS	4
1	B	212	GLU	4
1	A	116	ARG	4
1	A	234	GLU	4
1	B	116	ARG	4
1	B	167	SER	4
1	B	234	GLU	4
1	A	86	MET	4
1	A	201	SER	4
1	B	86	MET	4
1	B	201	SER	4
1	A	231	SER	4
1	B	98	GLN	4
1	B	231	SER	4
1	A	104	PHE	3
1	A	169	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	173	ARG	3
1	B	104	PHE	3
1	B	105	GLN	3
1	B	112	MET	3
1	B	169	GLU	3
1	B	173	ARG	3
1	A	88	LYS	3
1	A	90	LEU	3
1	A	195	LYS	3
1	A	226	LYS	3
1	A	240	LEU	3
1	B	88	LYS	3
1	B	90	LEU	3
1	B	195	LYS	3
1	B	226	LYS	3
1	B	240	LEU	3
1	A	87	SER	3
1	A	92	GLU	3
1	A	170	LEU	3
1	A	188	ARG	3
1	A	198	GLU	3
1	B	87	SER	3
1	B	92	GLU	3
1	B	188	ARG	3
1	B	198	GLU	3
1	A	102	ASP	3
1	B	102	ASP	3
1	A	106	LYS	2
1	A	114	LEU	2
1	A	199	HIS	2
1	A	223	GLU	2
1	A	229	PHE	2
1	B	106	LYS	2
1	B	114	LEU	2
1	B	146	GLU	2
1	B	199	HIS	2
1	B	223	GLU	2
1	B	229	PHE	2
1	A	77	LYS	2
1	A	96	LYS	2
1	A	153	ARG	2
1	A	162	HIS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	213	ASP	2
1	B	77	LYS	2
1	B	96	LYS	2
1	B	153	ARG	2
1	B	162	HIS	2
1	B	213	ASP	2
1	A	214	LEU	2
1	B	214	LEU	2
1	A	74	ASN	2
1	A	76	GLU	2
1	B	76	GLU	2
1	A	82	LEU	2
1	A	171	ARG	2
1	A	193	HIS	2
1	B	82	LEU	2
1	B	171	ARG	2
1	B	193	HIS	2
1	A	181	LEU	2
1	A	202	THR	2
1	A	203	LEU	2
1	B	170	LEU	2
1	B	181	LEU	2
1	B	202	THR	2
1	B	203	LEU	2
1	A	79	THR	2
1	A	149	ARG	2
1	B	79	THR	2
1	A	80	GLU	1
1	B	80	GLU	1
1	A	111	GLU	1
1	A	218	LEU	1
1	B	111	GLU	1
1	B	218	LEU	1
1	A	117	GLN	1
1	A	118	LYS	1
1	B	117	GLN	1
1	B	118	LYS	1
1	B	149	ARG	1
1	A	225	PHE	1
1	A	241	ASN	1
1	B	74	ASN	1
1	B	225	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	B	241	ASN	1
1	A	211	LEU	1
1	B	211	LEU	1
1	A	109	GLN	1
1	B	109	GLN	1
1	A	83	ARG	1
1	B	83	ARG	1
1	A	110	GLU	1
1	B	110	GLU	1
1	A	94	LYS	1
1	A	160	ARG	1
1	B	94	LYS	1
1	B	160	ARG	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 oligosaccharides 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 15% for the well-defined parts and 15% 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	689
Number of shifts mapped to atoms	689
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
$^{13}\text{C}_\alpha$	159	-0.32 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	83	1.10 ± 0.08	Should be checked
$^{13}\text{C}'$	149	1.87 ± 0.06	Should be applied
^{15}N	149	-0.00 ± 0.08	None needed (< 0.5 ppm)

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 15%, i.e. 606 atoms were assigned a chemical shift out of a possible 4154. 0 out of 58 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	537/1450 (37%)	132/584 (23%)	273/584 (47%)	132/282 (47%)
Sidechain	69/2474 (3%)	0/1588 (0%)	69/772 (9%)	0/114 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/230 (0%)	0/114 (0%)	0/106 (0%)	0/10 (0%)
Overall	606/4154 (15%)	132/2286 (6%)	342/1462 (23%)	132/406 (33%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 15%, i.e. 689 atoms were assigned a chemical shift out of a possible 4740. 0 out of 64 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	606/1658 (37%)	149/668 (22%)	308/668 (46%)	149/322 (46%)
Sidechain	83/2788 (3%)	0/1788 (0%)	83/872 (10%)	0/128 (0%)
Aromatic	0/294 (0%)	0/146 (0%)	0/136 (0%)	0/12 (0%)
Overall	689/4740 (15%)	149/2602 (6%)	391/1676 (23%)	149/462 (32%)

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. 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:

