



Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 04:09 PM EST

PDB ID : 2N5E
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

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

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20028442
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

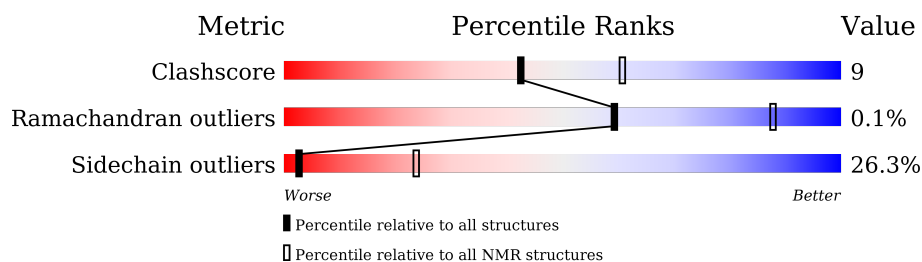
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 16%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 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)	0.76	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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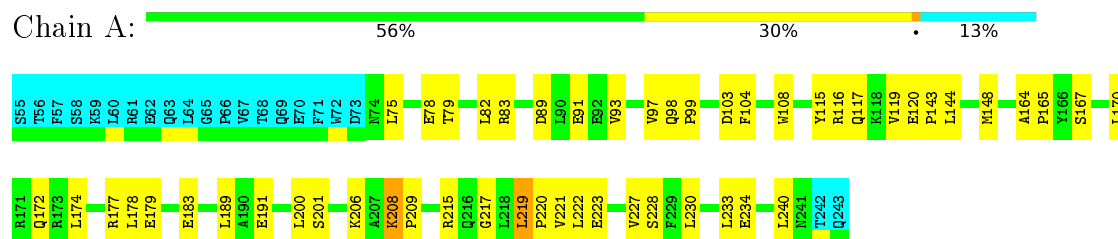
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	DELETION	UNP P02647
B	?	-	GLY	DELETION	UNP P02647
B	?	-	ALA	DELETION	UNP P02647
B	?	-	ARG	DELETION	UNP P02647
B	?	-	GLN	DELETION	UNP P02647
B	?	-	LYS	DELETION	UNP P02647
B	?	-	LEU	DELETION	UNP P02647
B	?	-	HIS	DELETION	UNP P02647
B	?	-	GLU	DELETION	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

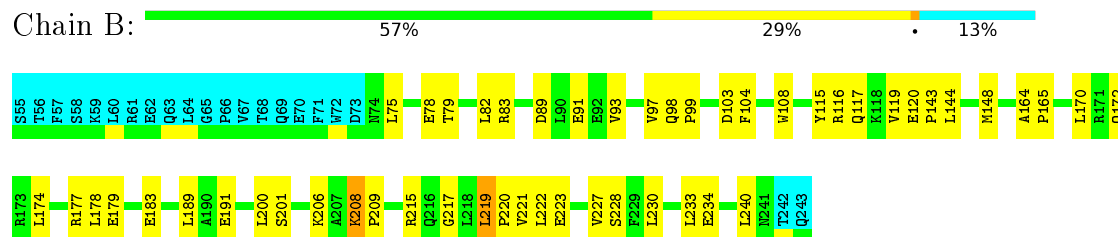
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA 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: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I

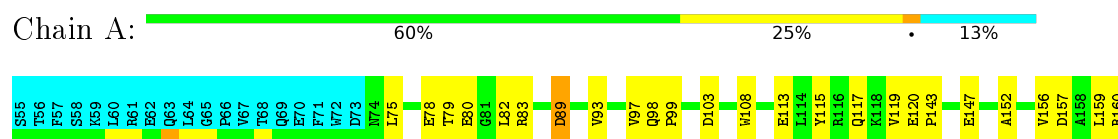


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

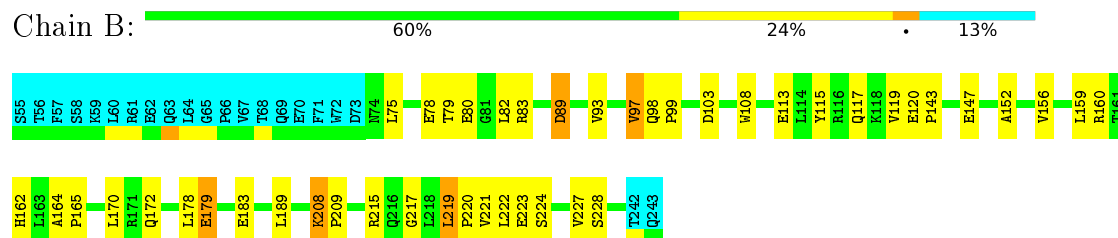
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Apolipoprotein A-I



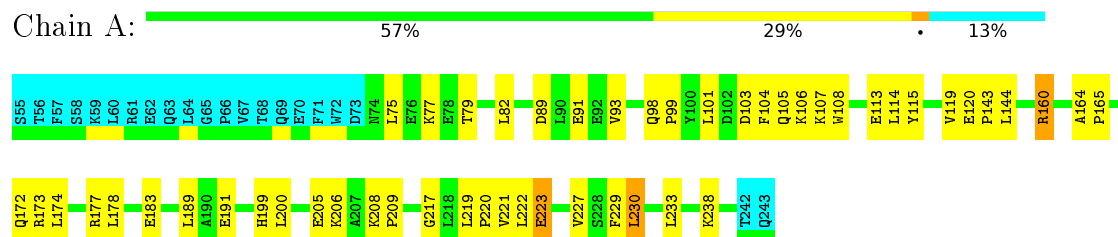


• Molecule 1: Apolipoprotein A-I

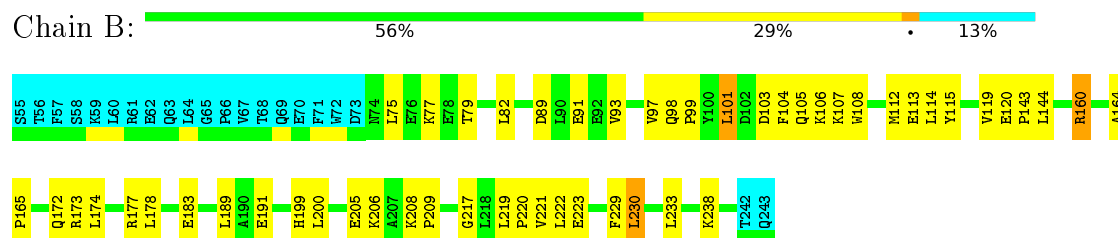


4.2.2 Score per residue for model 2

• Molecule 1: Apolipoprotein A-I

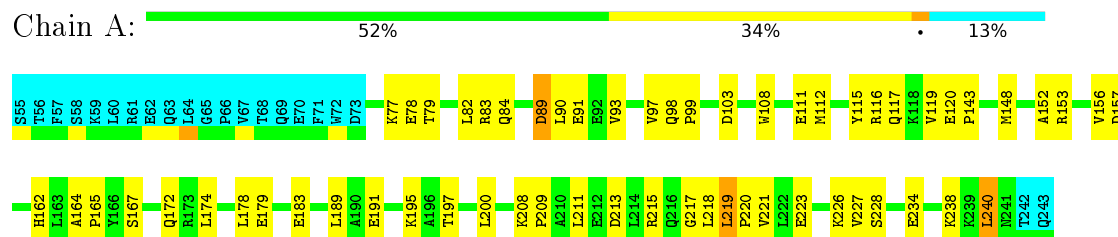


• Molecule 1: Apolipoprotein A-I

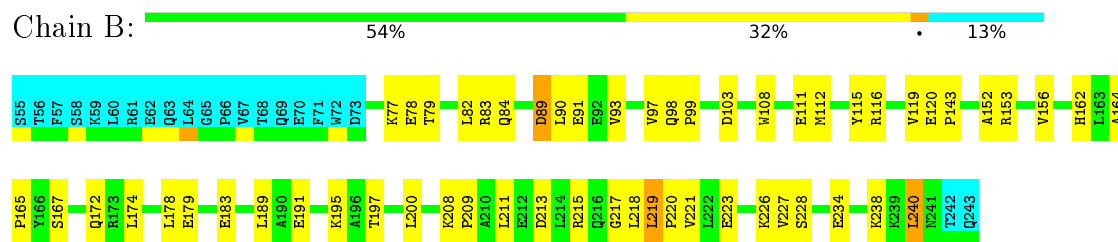


4.2.3 Score per residue for model 3

• Molecule 1: Apolipoprotein A-I

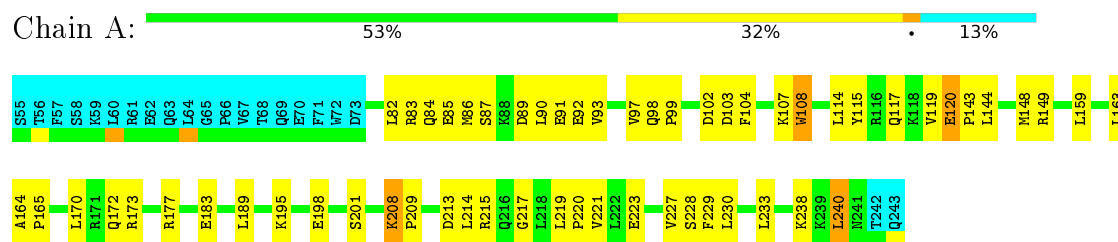


• Molecule 1: Apolipoprotein A-I

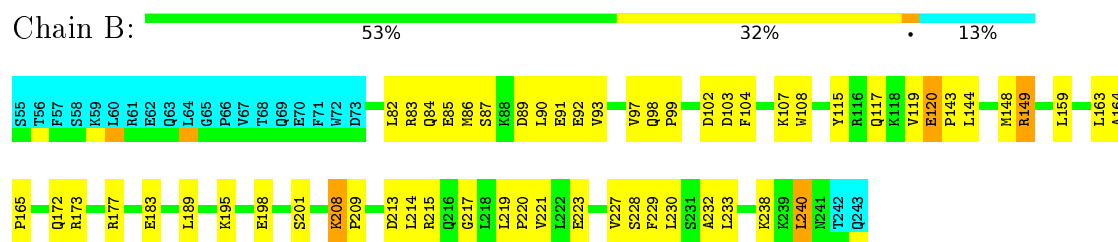


4.2.4 Score per residue for model 4

- Molecule 1: Apolipoprotein A-I

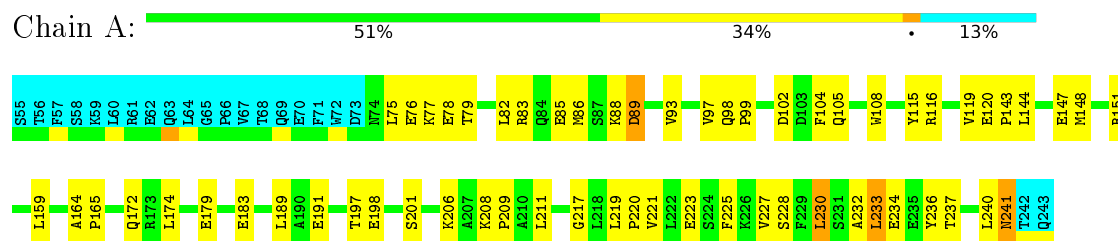


- Molecule 1: Apolipoprotein A-I

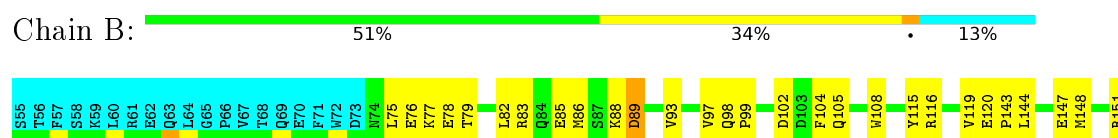


4.2.5 Score per residue for model 5

- Molecule 1: Apolipoprotein A-I



- Molecule 1: Apolipoprotein A-I



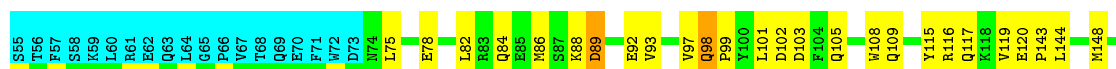


4.2.6 Score per residue for model 6

- Molecule 1: Apolipoprotein A-I

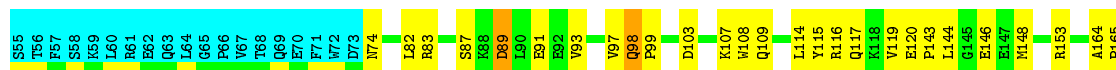


- Molecule 1: Apolipoprotein A-I



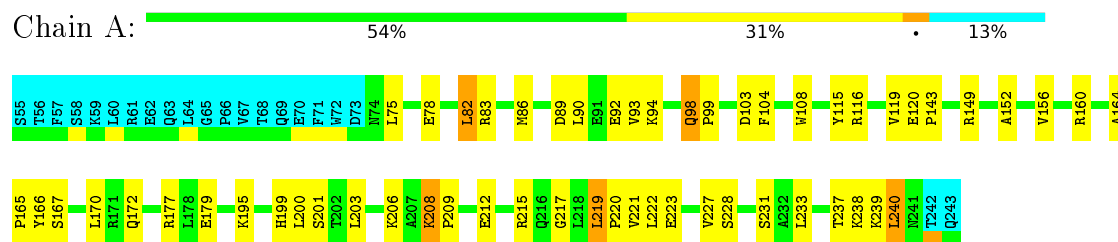
4.2.7 Score per residue for model 7

- Molecule 1: Apolipoprotein A-I

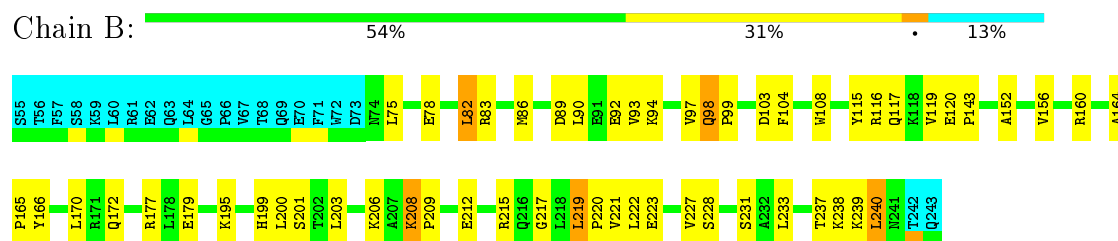


- Molecule 1: Apolipoprotein A-I





- 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)	2n5e_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)	16%

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	1192	1198	1198	22±2
1	B	1192	1198	1198	21±2
All	All	23840	23960	23960	414

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:B:164:ALA:HB3	1:B:165:PRO:CD	0.64	2.23	3	10
1:A:164:ALA:HB3	1:A:165:PRO:CD	0.64	2.23	7	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:O	1:B:82:LEU:HD13	0.58	1.99	5	3
1:A:82:LEU:HD13	1:A:82:LEU:O	0.58	1.99	5	2
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: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
1:A:217:GLY:O	1:A:221:VAL:HG23	0.50	2.07	2	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:170:LEU:C	1:A:170:LEU:HD13	0.48	2.29	4	3
1:B:98:GLN:CB	1:B:99:PRO:HD3	0.47	2.38	8	10
1:A:93:VAL:O	1:A:97:VAL:HG23	0.47	2.09	9	7
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: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:HD13	1:B:240:LEU:O	0.47	2.09	4	1
1:A:197:THR:HG21	1:B:240:LEU:HD22	0.46	1.87	3	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:HD13	1:B:230:LEU:O	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:82:LEU:O	1:A:82:LEU:HD13	0.44	2.11	6	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
1:B:170:LEU:HD13	1:B:170:LEU:C	0.44	2.33	1	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:B:79:THR:O	1:B:82:LEU:HD23	0.42	2.14	2	2
1:A:208:LYS:N	1:A:209:PRO:HD2	0.42	2.28	2	2
1:A:211:LEU:C	1:A:211:LEU:HD13	0.42	2.35	5	1
1:B:230:LEU:HD13	1:B:230:LEU:C	0.42	2.35	7	1
1:A:170:LEU:O	1:A:170:LEU:HD22	0.42	2.14	4	1
1:A:230:LEU:HD13	1:A:230:LEU:C	0.42	2.35	7	1
1:B:114:LEU:HD13	1:B:114:LEU:C	0.42	2.35	8	1
1:A:156:VAL:CG1	1:A:157:ASP:N	0.42	2.83	8	1
1:A:114:LEU:HD13	1:A:114:LEU:C	0.42	2.35	8	1
1:B:170:LEU:C	1:B:170:LEU:HD13	0.41	2.35	6	1
1:A:211:LEU:HD13	1:A:211:LEU:C	0.41	2.35	3	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:B:211:LEU:C	1:B:211:LEU:HD13	0.41	2.35	3	2
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:O	1:B:170:LEU:HD22	0.41	2.16	1	1
1:B:208:LYS:CB	1:B:209:PRO:HD3	0.41	2.46	8	2
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%)	59	88
1	B	146/167 (87%)	141±1 (97±1%)	5±1 (3±1%)	0±0 (0±0%)	59	88

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2920/3340 (87%)	2824 (97%)	94 (3%)	2 (0%)	59 88

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	B	241	ASN	1
1	A	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%)	93±5 (74±4%)	33±5 (26±4%)	3 24
1	B	126/146 (86%)	93±4 (74±3%)	33±4 (26±3%)	3 24
All	All	2520/2920 (86%)	1857 (74%)	663 (26%)	3 24

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	B	172	GLN	10
1	A	108	TRP	10
1	A	172	GLN	10
1	B	108	TRP	9
1	B	183	GLU	8
1	A	189	LEU	8
1	B	189	LEU	8
1	A	103	ASP	8
1	B	103	ASP	8
1	A	183	GLU	8
1	B	144	LEU	7
1	A	144	LEU	7
1	B	233	LEU	6
1	A	208	LYS	6
1	A	148	MET	6

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Mol	Chain	Res	Type	Models (Total)
1	A	228	SER	6
1	B	208	LYS	6
1	A	233	LEU	6
1	B	228	SER	6
1	B	104	PHE	6
1	A	219	LEU	5
1	B	177	ARG	5
1	B	174	LEU	5
1	A	167	SER	5
1	B	222	LEU	5
1	A	206	LYS	5
1	A	215	ARG	5
1	B	89	ASP	5
1	A	200	LEU	5
1	B	91	GLU	5
1	A	174	LEU	5
1	B	83	ARG	5
1	B	206	LYS	5
1	B	78	GLU	5
1	B	148	MET	5
1	B	219	LEU	5
1	A	104	PHE	5
1	A	116	ARG	5
1	A	177	ARG	5
1	B	191	GLU	5
1	B	116	ARG	5
1	A	222	LEU	5
1	B	200	LEU	5
1	A	89	ASP	5
1	A	191	GLU	5
1	A	78	GLU	5
1	A	91	GLU	5
1	A	83	ARG	5
1	B	215	ARG	5
1	B	173	ARG	4
1	B	75	LEU	4
1	B	98	GLN	4
1	A	75	LEU	4
1	B	167	SER	4
1	A	86	MET	4
1	A	239	LYS	4
1	A	84	GLN	4

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Mol	Chain	Res	Type	Models (Total)
1	B	230	LEU	4
1	A	230	LEU	4
1	B	102	ASP	4
1	A	231	SER	4
1	A	102	ASP	4
1	B	234	GLU	4
1	B	231	SER	4
1	B	224	SER	4
1	A	98	GLN	4
1	B	120	GLU	4
1	B	239	LYS	4
1	A	226	LYS	4
1	A	77	LYS	4
1	A	173	ARG	4
1	A	179	GLU	4
1	B	86	MET	4
1	A	224	SER	4
1	B	238	LYS	4
1	A	201	SER	4
1	B	77	LYS	4
1	B	226	LYS	4
1	B	179	GLU	4
1	B	84	GLN	4
1	A	234	GLU	4
1	A	238	LYS	4
1	B	201	SER	4
1	A	162	HIS	3
1	A	160	ARG	3
1	B	229	PHE	3
1	A	105	GLN	3
1	A	147	GLU	3
1	A	159	LEU	3
1	A	198	GLU	3
1	A	85	GLU	3
1	A	240	LEU	3
1	B	105	GLN	3
1	A	182	LYS	3
1	B	171	ARG	3
1	B	182	LYS	3
1	B	159	LEU	3
1	B	160	ARG	3
1	A	149	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	A	195	LYS	3
1	B	97	VAL	3
1	A	88	LYS	3
1	B	90	LEU	3
1	B	195	LYS	3
1	A	92	GLU	3
1	A	171	ARG	3
1	A	87	SER	3
1	B	87	SER	3
1	B	107	LYS	3
1	B	198	GLU	3
1	B	240	LEU	3
1	B	112	MET	3
1	A	90	LEU	3
1	B	85	GLU	3
1	B	162	HIS	3
1	A	107	LYS	3
1	B	92	GLU	3
1	A	229	PHE	3
1	A	114	LEU	3
1	A	120	GLU	3
1	B	101	LEU	3
1	B	88	LYS	3
1	B	147	GLU	3
1	A	212	GLU	2
1	A	170	LEU	2
1	B	149	ARG	2
1	B	223	GLU	2
1	A	109	GLN	2
1	A	112	MET	2
1	B	114	LEU	2
1	A	223	GLU	2
1	A	169	GLU	2
1	A	188	ARG	2
1	A	79	THR	2
1	A	202	THR	2
1	A	76	GLU	2
1	A	193	HIS	2
1	A	213	ASP	2
1	B	193	HIS	2
1	B	225	PHE	2
1	A	203	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	199	HIS	2
1	B	109	GLN	2
1	B	113	GLU	2
1	A	146	GLU	2
1	A	94	LYS	2
1	B	202	THR	2
1	B	94	LYS	2
1	B	212	GLU	2
1	B	214	LEU	2
1	B	213	ASP	2
1	A	214	LEU	2
1	B	76	GLU	2
1	A	101	LEU	2
1	A	153	ARG	2
1	B	199	HIS	2
1	B	188	ARG	2
1	B	170	LEU	2
1	B	169	GLU	2
1	B	203	LEU	2
1	B	153	ARG	2
1	A	113	GLU	2
1	B	79	THR	2
1	A	225	PHE	2
1	A	74	ASN	1
1	B	151	ARG	1
1	B	111	GLU	1
1	B	110	GLU	1
1	B	157	ASP	1
1	A	97	VAL	1
1	B	211	LEU	1
1	B	106	LYS	1
1	B	178	LEU	1
1	A	111	GLU	1
1	A	157	ASP	1
1	B	146	GLU	1
1	A	151	ARG	1
1	A	82	LEU	1
1	B	80	GLU	1
1	B	181	LEU	1
1	A	80	GLU	1
1	A	218	LEU	1
1	A	106	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	B	241	ASN	1
1	A	117	GLN	1
1	B	82	LEU	1
1	A	178	LEU	1
1	B	205	GLU	1
1	A	211	LEU	1
1	A	181	LEU	1
1	A	241	ASN	1
1	A	110	GLU	1
1	A	205	GLU	1
1	B	218	LEU	1
1	B	117	GLN	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 carbohydrates in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

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

The completeness of assignment taking into account all chemical shift lists is 16% for the well-defined parts and 16% for the entire structure.

7.1 Chemical shift list 1

File name: 2n5e_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	-0.33 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	83	1.09 ± 0.07	Should be applied
$^{13}\text{C}'$	149	1.86 ± 0.06	Should be applied
^{15}N	149	0.00 ± 0.12	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 16%, i.e. 606 atoms were assigned a chemical shift out of a possible 3804. 0 out of 58 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	537/1440 (37%)	132/574 (23%)	273/584 (47%)	132/282 (47%)
Sidechain	69/2150 (3%)	0/1264 (0%)	69/772 (9%)	0/114 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/214 (0%)	0/114 (0%)	0/90 (0%)	0/10 (0%)
Overall	606/3804 (16%)	132/1952 (7%)	342/1446 (24%)	132/406 (33%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 16%, i.e. 689 atoms were assigned a chemical shift out of a possible 4348. 0 out of 64 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	606/1646 (37%)	149/656 (23%)	308/668 (46%)	149/322 (46%)
Sidechain	83/2428 (3%)	0/1428 (0%)	83/872 (10%)	0/128 (0%)
Aromatic	0/274 (0%)	0/146 (0%)	0/116 (0%)	0/12 (0%)
Overall	689/4348 (16%)	149/2230 (7%)	391/1656 (24%)	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.

Random coil index (RCI) for chain A:

