



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 11:24 AM UTC

PDB ID : 1YS5 / pdb_00001ys5
Title : Solution structure of the antigenic domain of GNA1870 of Neisseria meningitidis
Authors : Cantini, F.; Savino, S.; Massignani, V.; Pizza, M.; Scarselli, M.; Swennen, E.; Romagnoli, G.; Veggi, D.; Banci, L.; Rappuoli, R.
Deposited on : 2005-02-07

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 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

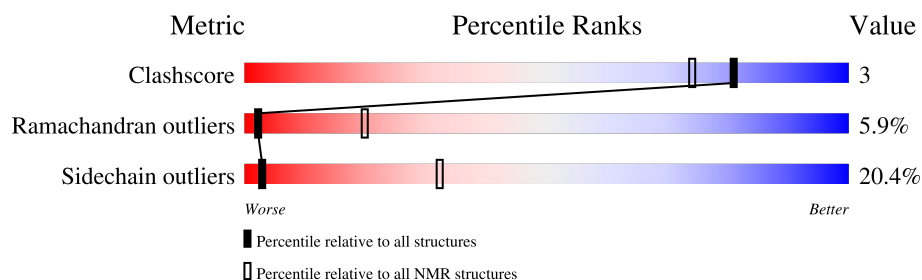
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	164	56% 17% 22% 5%

2 Ensemble composition and analysis

This entry contains 30 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 12 as representative, based on the following criterion: *closest to the average*.

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:37-A:156 (120)	1.13	17

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 24 single-model clusters were found.

Cluster number	Models
1	4, 25
2	5, 30
3	3, 18
Single-model clusters	1; 2; 6; 7; 8; 9; 10; 11; 12; 13; 14; 15; 16; 17; 19; 20; 21; 22; 23; 24; 26; 27; 28; 29

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2313 atoms, of which 1149 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called lipoprotein.

Mol	Chain	Residues	Atoms						Trace
1	A	156	Total	C	H	N	O	S	0
			2313	721	1149	212	229	2	

There are 9 discrepancies between the modelled and reference sequences:

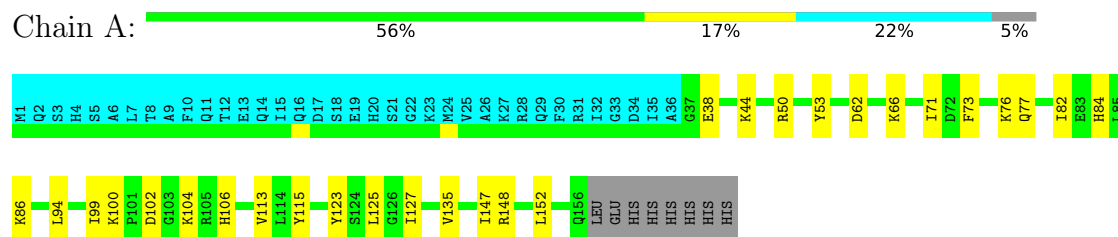
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	GB 46562309
A	157	LEU	-	expression tag	GB 46562309
A	158	GLU	-	expression tag	GB 46562309
A	159	HIS	-	expression tag	GB 46562309
A	160	HIS	-	expression tag	GB 46562309
A	161	HIS	-	expression tag	GB 46562309
A	162	HIS	-	expression tag	GB 46562309
A	163	HIS	-	expression tag	GB 46562309
A	164	HIS	-	expression tag	GB 46562309

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: lipoprotein

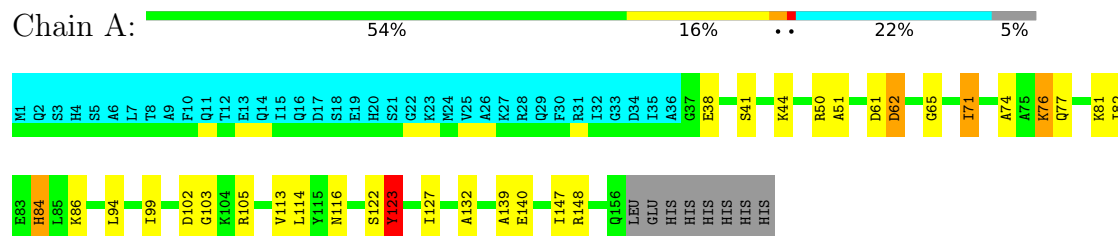


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

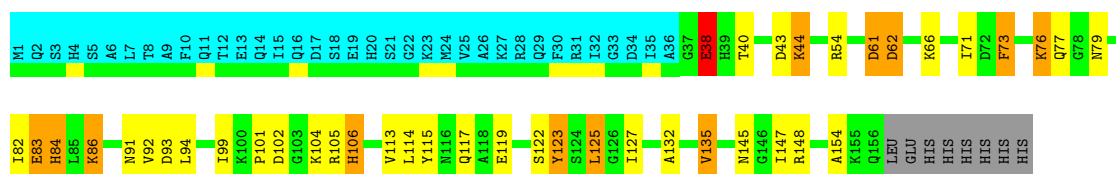
- Molecule 1: lipoprotein



4.2.2 Score per residue for model 2

- Molecule 1: lipoprotein

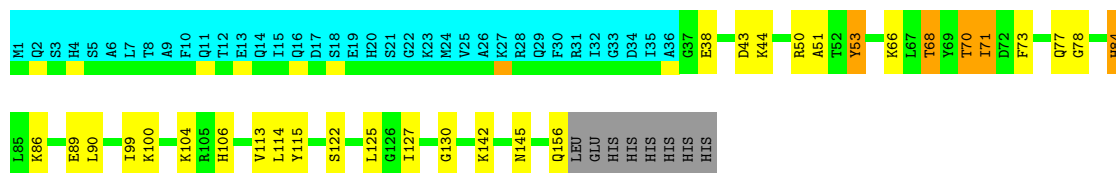




4.2.3 Score per residue for model 3

- Molecule 1: lipoprotein

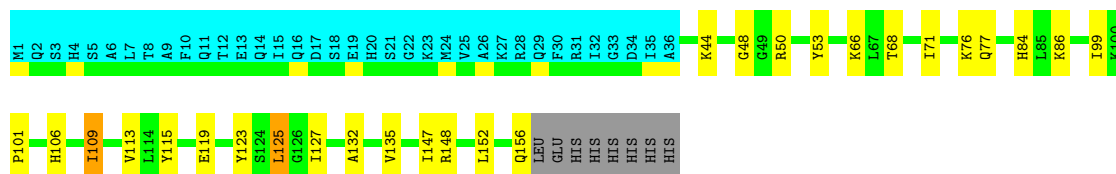
Chain A: 54% 16% 22% 5%



4.2.4 Score per residue for model 4

- Molecule 1: lipoprotein

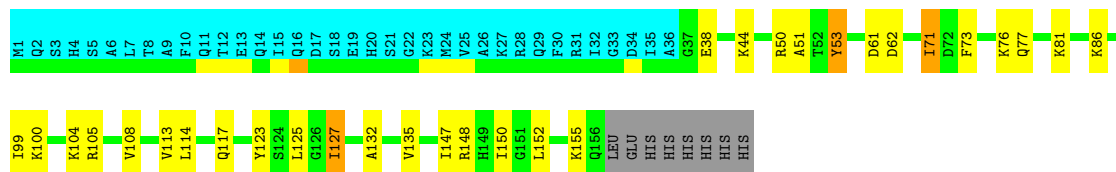
Chain A: 57% 15% 22% 5%



4.2.5 Score per residue for model 5

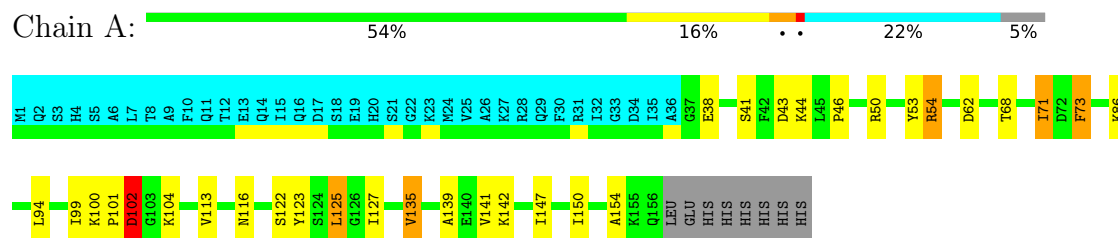
- Molecule 1: lipoprotein

Chain A: 54% 17% 22% 5%



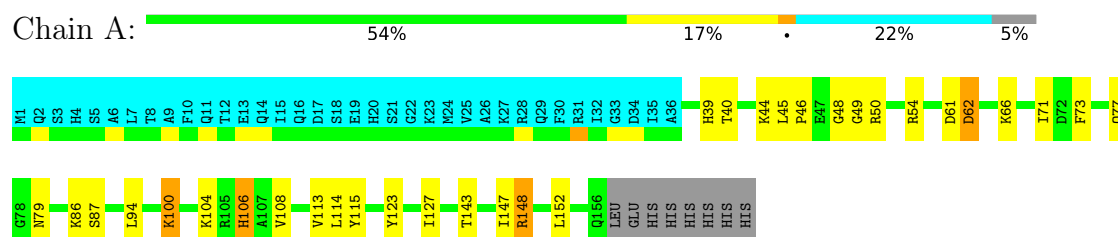
4.2.6 Score per residue for model 6

- Molecule 1: lipoprotein



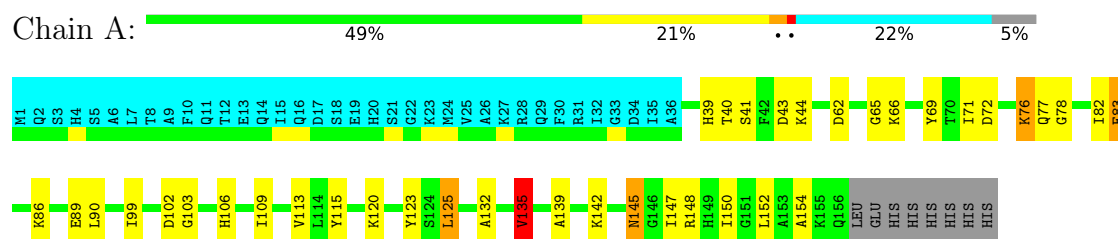
4.2.7 Score per residue for model 7

- Molecule 1: lipoprotein



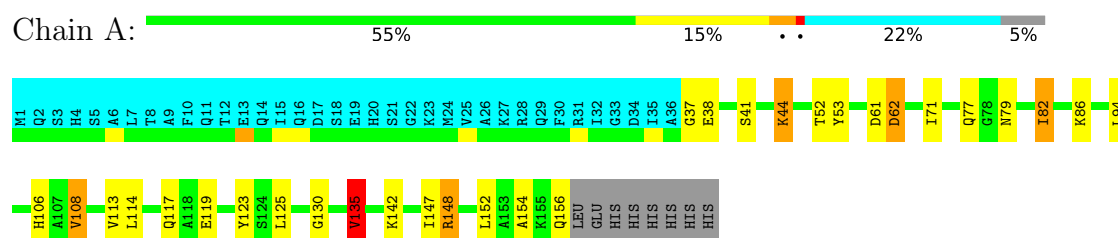
4.2.8 Score per residue for model 8

- Molecule 1: lipoprotein



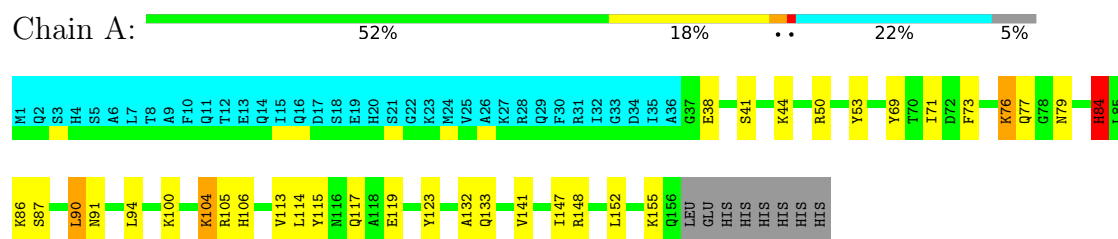
4.2.9 Score per residue for model 9

- Molecule 1: lipoprotein



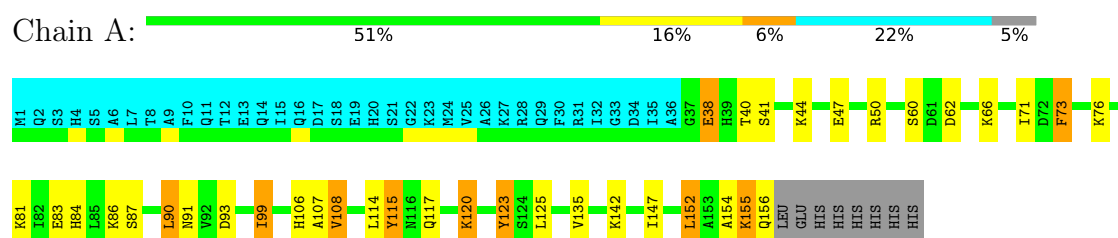
4.2.10 Score per residue for model 10

- Molecule 1: lipoprotein



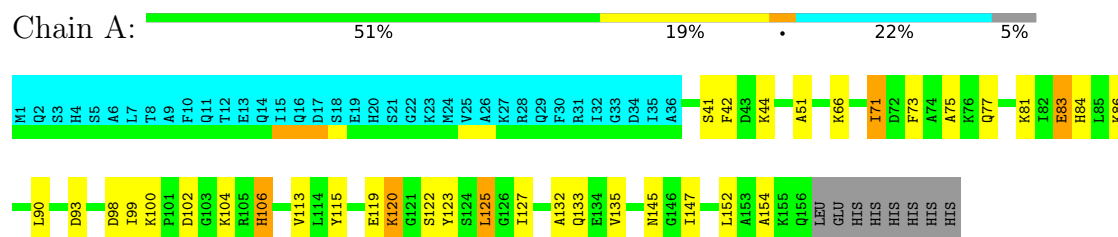
4.2.11 Score per residue for model 11

- Molecule 1: lipoprotein



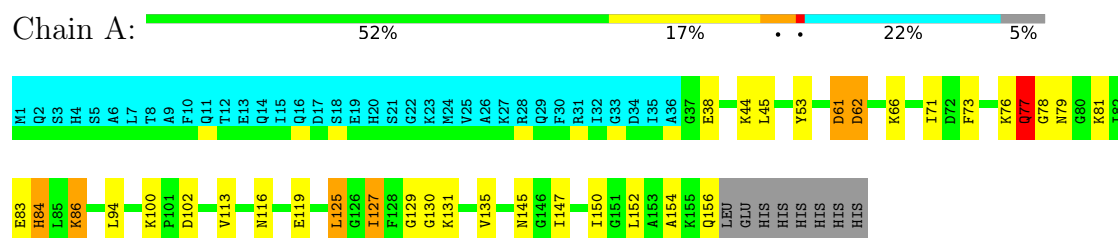
4.2.12 Score per residue for model 12

- Molecule 1: lipoprotein



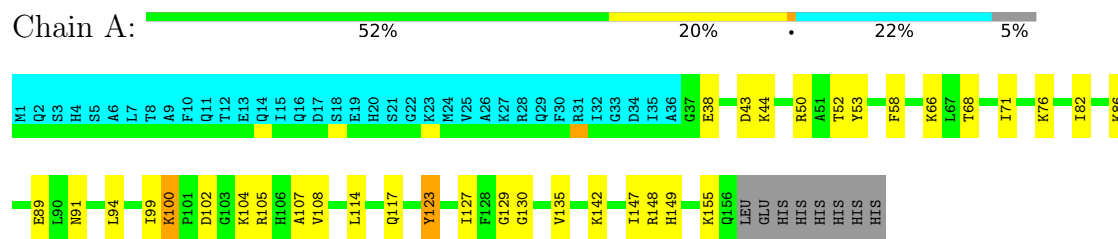
4.2.13 Score per residue for model 13

- Molecule 1: lipoprotein



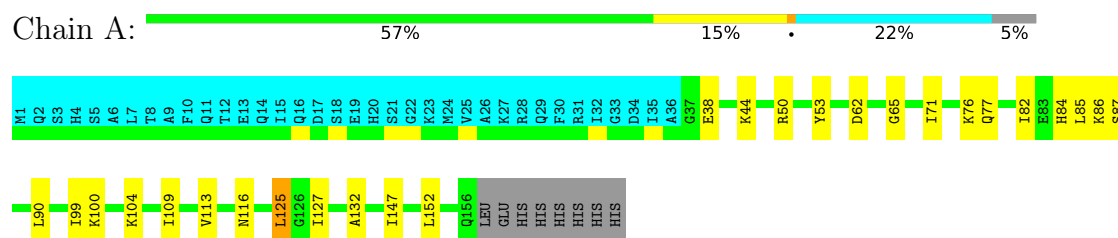
4.2.14 Score per residue for model 14

- Molecule 1: lipoprotein



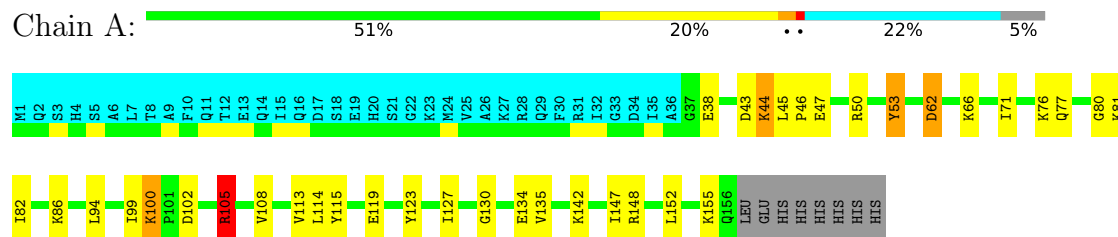
4.2.15 Score per residue for model 15

- Molecule 1: lipoprotein



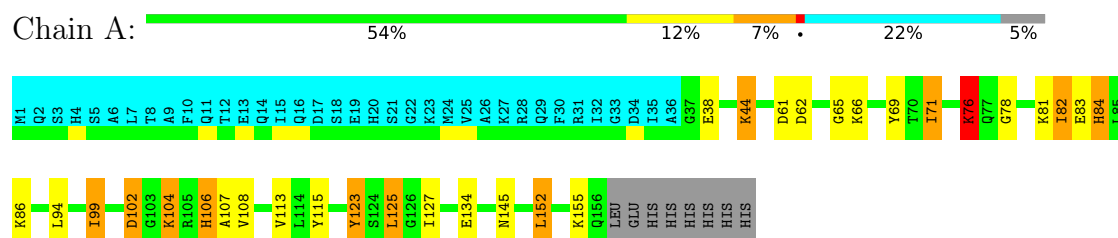
4.2.16 Score per residue for model 16

- Molecule 1: lipoprotein



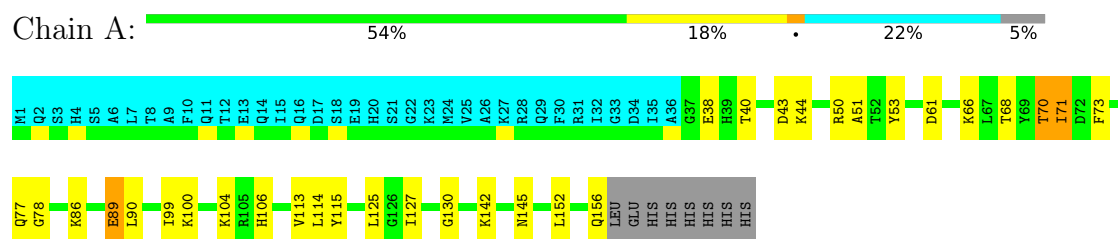
4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: lipoprotein



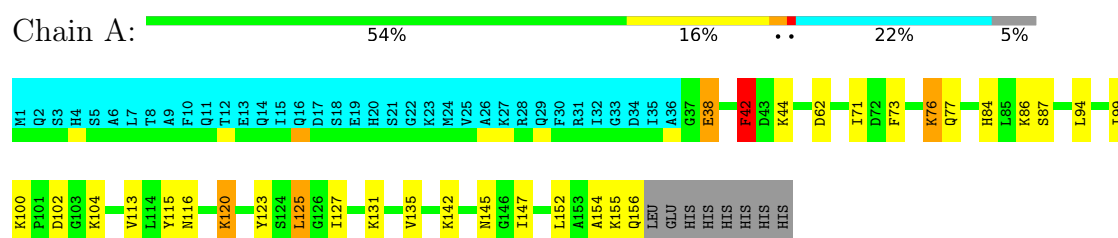
4.2.18 Score per residue for model 18

- Molecule 1: lipoprotein



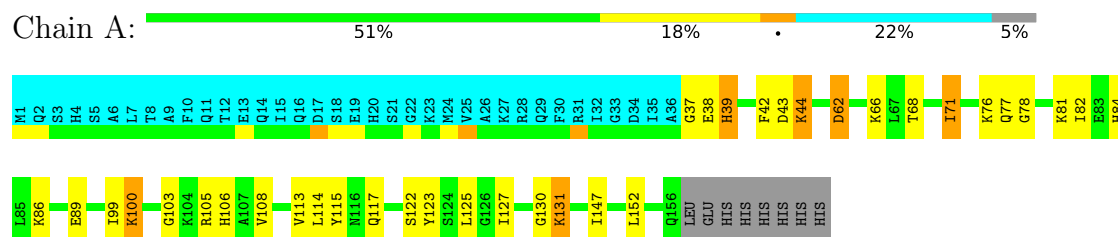
4.2.19 Score per residue for model 19

- Molecule 1: lipoprotein



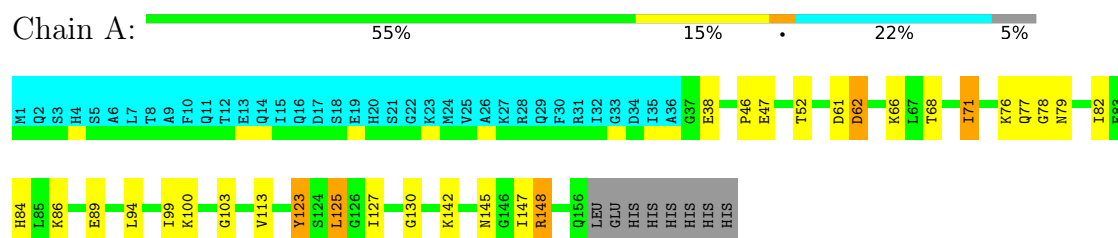
4.2.20 Score per residue for model 20

- Molecule 1: lipoprotein



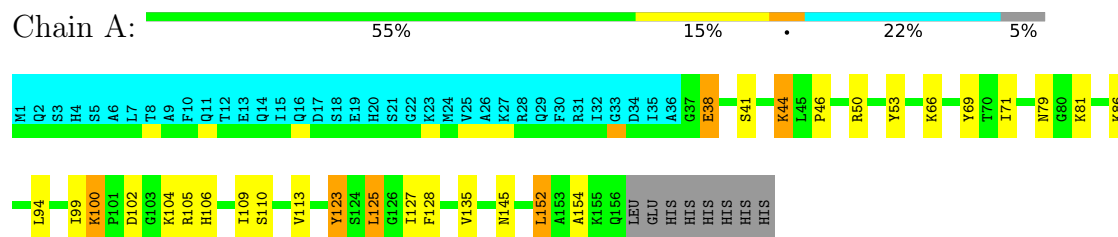
4.2.21 Score per residue for model 21

- Molecule 1: lipoprotein



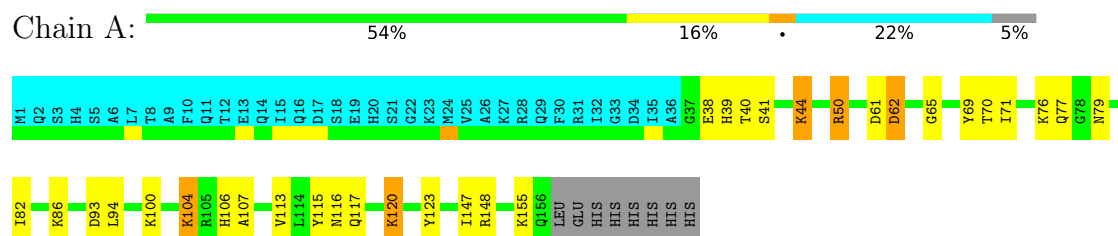
4.2.22 Score per residue for model 22

- Molecule 1: lipoprotein



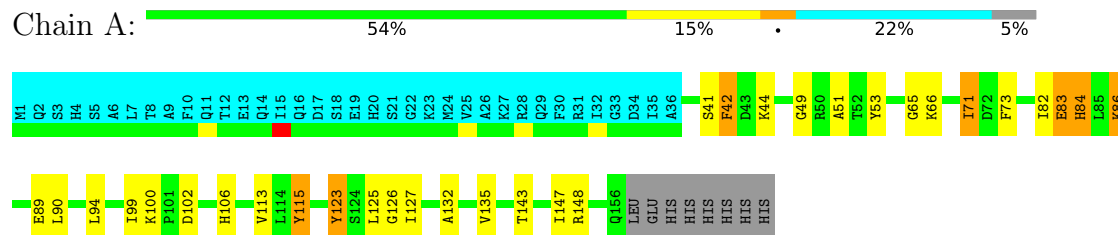
4.2.23 Score per residue for model 23

- Molecule 1: lipoprotein



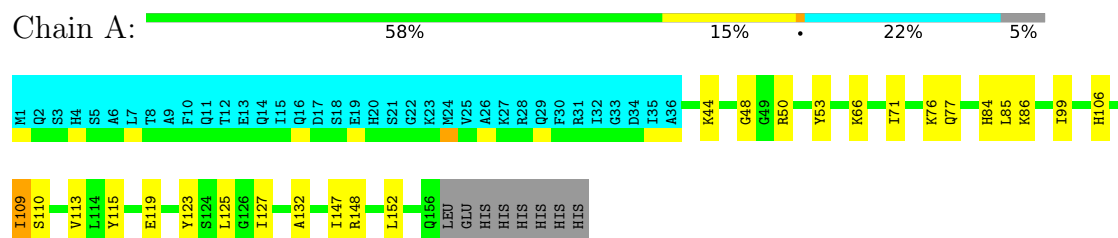
4.2.24 Score per residue for model 24

- Molecule 1: lipoprotein



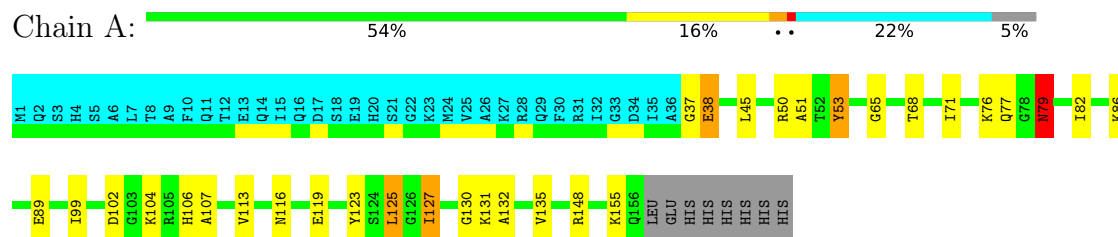
4.2.25 Score per residue for model 25

- Molecule 1: lipoprotein



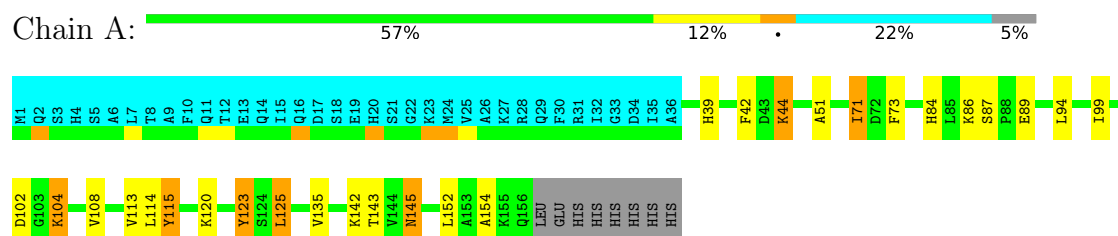
4.2.26 Score per residue for model 26

- Molecule 1: lipoprotein



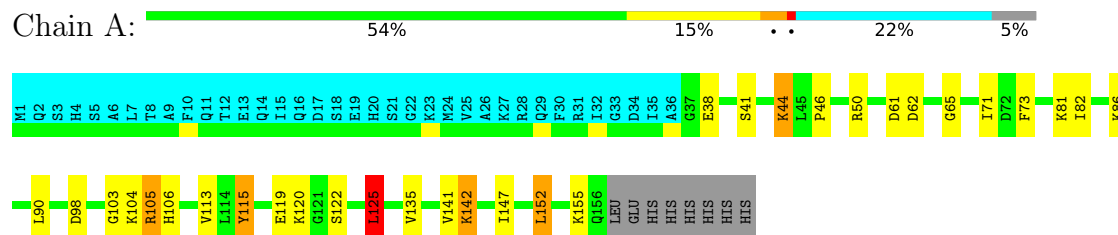
4.2.27 Score per residue for model 27

- Molecule 1: lipoprotein



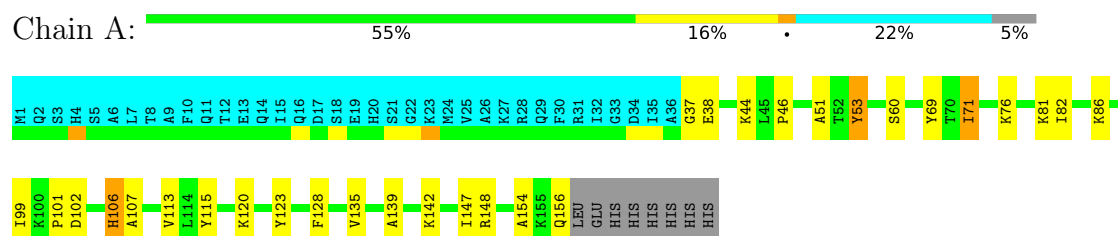
4.2.28 Score per residue for model 28

- Molecule 1: lipoprotein



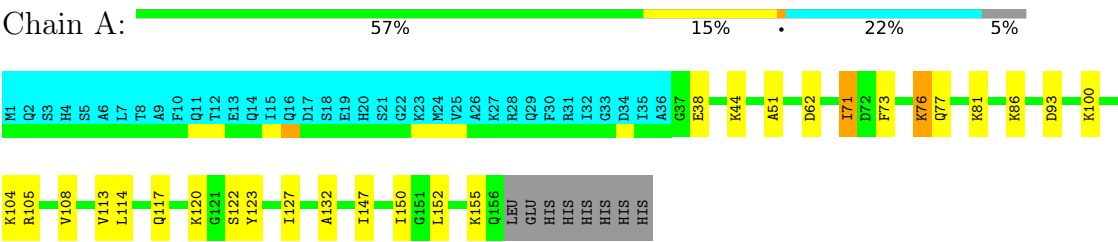
4.2.29 Score per residue for model 29

- Molecule 1: lipoprotein



4.2.30 Score per residue for model 30

● Molecule 1: lipoprotein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, simulated annealing*.

Of the 400 calculated structures, 30 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
DYANA	structure solution	1.5
CANDID	structure solution	2
Amber	refinement	5.0

No chemical shift data was provided.

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	0.63±0.01	0±0/896 (0.0± 0.0%)	1.34±0.03	3±2/1203 (0.2± 0.2%)
All	All	0.63	0/26880 (0.0%)	1.34	90/36090 (0.2%)

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	4.9±1.8
All	All	0	148

There are no bond-length outliers.

All 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
1	A	102	ASP	CA-CB-CG	9.84	122.44	112.60	6	2
1	A	125	LEU	CA-C-N	7.32	130.47	121.83	3	11
1	A	125	LEU	C-N-CA	7.32	130.47	121.83	3	11
1	A	106	HIS	CA-CB-CG	7.09	120.89	113.80	12	3
1	A	79	ASN	CA-CB-CG	-6.76	105.84	112.60	26	1
1	A	135	VAL	CA-CB-CG2	6.52	121.48	110.40	8	2
1	A	83	GLU	CA-C-N	6.49	133.38	121.70	8	3
1	A	83	GLU	C-N-CA	6.49	133.38	121.70	8	3
1	A	106	HIS	CB-CG-CD2	-6.38	122.90	131.20	26	6
1	A	84	HIS	CB-CG-CD2	-6.34	122.96	131.20	10	4
1	A	130	GLY	CA-C-N	6.09	133.17	121.54	26	2
1	A	130	GLY	C-N-CA	6.09	133.17	121.54	26	2
1	A	76	LYS	CB-CA-C	5.92	119.69	111.63	10	1
1	A	108	VAL	N-CA-C	5.90	116.14	108.35	14	2
1	A	145	ASN	CA-CB-CG	5.89	118.49	112.60	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	82	ILE	CA-CB-CG2	5.47	119.80	110.50	16	1
1	A	39	HIS	CB-CG-CD2	-5.42	124.15	131.20	27	1
1	A	45	LEU	CA-C-N	5.38	126.56	119.84	16	1
1	A	45	LEU	C-N-CA	5.38	126.56	119.84	16	1
1	A	41	SER	CA-C-N	5.37	127.74	120.38	28	3
1	A	41	SER	C-N-CA	5.37	127.74	120.38	28	3
1	A	43	ASP	CA-C-N	5.30	131.67	121.54	6	2
1	A	43	ASP	C-N-CA	5.30	131.67	121.54	6	2
1	A	73	PHE	CA-CB-CG	5.30	119.10	113.80	6	2
1	A	99	ILE	CB-CA-C	5.27	118.68	112.68	11	1
1	A	108	VAL	CB-CA-C	-5.21	106.84	111.74	30	2
1	A	84	HIS	CA-CB-CG	5.15	118.95	113.80	24	1
1	A	107	ALA	CA-C-N	5.15	127.12	121.97	11	1
1	A	107	ALA	C-N-CA	5.15	127.12	121.97	11	1
1	A	72	ASP	CA-C-N	5.10	127.42	120.54	8	1
1	A	72	ASP	C-N-CA	5.10	127.42	120.54	8	1
1	A	120	LYS	CB-CA-C	5.10	118.72	111.74	12	1
1	A	108	VAL	CA-C-N	5.09	127.71	122.27	20	2
1	A	108	VAL	C-N-CA	5.09	127.71	122.27	20	2
1	A	82	ILE	CA-CB-CG1	5.07	119.02	110.40	9	1
1	A	71	ILE	CB-CA-C	5.05	116.74	110.73	6	1
1	A	85	LEU	CA-C-N	5.03	131.15	121.54	25	1
1	A	85	LEU	C-N-CA	5.03	131.15	121.54	25	1
1	A	40	THR	CA-C-N	5.02	128.35	120.82	18	1
1	A	40	THR	C-N-CA	5.02	128.35	120.82	18	1
1	A	42	PHE	CA-CB-CG	5.00	118.80	113.80	19	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	123	TYR	Sidechain	19
1	A	53	TYR	Sidechain,Peptide	14
1	A	115	TYR	Sidechain	14
1	A	73	PHE	Sidechain	12
1	A	61	ASP	Peptide	11
1	A	62	ASP	Peptide	11
1	A	84	HIS	Sidechain,Peptide	9
1	A	119	GLU	Peptide	8
1	A	148	ARG	Sidechain	8

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	69	TYR	Sidechain	6
1	A	105	ARG	Sidechain,Peptide	4
1	A	83	GLU	Peptide	4
1	A	50	ARG	Sidechain	3
1	A	68	THR	Peptide	3
1	A	42	PHE	Sidechain	3
1	A	54	ARG	Sidechain	2
1	A	70	THR	Peptide	2
1	A	120	LYS	Peptide	2
1	A	128	PHE	Sidechain	2
1	A	101	PRO	Peptide	1
1	A	108	VAL	Peptide	1
1	A	71	ILE	Peptide	1
1	A	104	LYS	Peptide	1
1	A	77	GLN	Peptide	1
1	A	155	LYS	Peptide	1
1	A	82	ILE	Peptide	1
1	A	98	ASP	Peptide	1
1	A	106	HIS	Sidechain	1
1	A	139	ALA	Peptide	1

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	882	872	872	4±2
All	All	26460	26160	26160	135

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.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:TYR:CE1	1:A:135:VAL:HG11	0.71	2.21	26	1
1:A:135:VAL:HG22	1:A:154:ALA:CB	0.71	2.16	8	6
1:A:135:VAL:HG22	1:A:154:ALA:HB3	0.69	1.62	11	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:VAL:HG22	1:A:142:LYS:H	0.66	1.51	28	1
1:A:65:GLY:HA3	1:A:82:ILE:HG23	0.64	1.69	15	8
1:A:53:TYR:CZ	1:A:135:VAL:HG13	0.62	2.30	16	1
1:A:125:LEU:HD13	1:A:126:GLY:N	0.61	2.10	24	1
1:A:135:VAL:CG2	1:A:154:ALA:HB3	0.59	2.27	19	2
1:A:53:TYR:CZ	1:A:71:ILE:HG21	0.58	2.33	18	2
1:A:109:ILE:HD12	1:A:109:ILE:C	0.58	2.24	25	3
1:A:71:ILE:HG22	1:A:78:GLY:HA2	0.57	1.77	3	4
1:A:51:ALA:HB2	1:A:71:ILE:HG13	0.57	1.77	29	1
1:A:139:ALA:HB3	1:A:150:ILE:CG2	0.56	2.31	6	1
1:A:125:LEU:C	1:A:125:LEU:HD13	0.55	2.27	15	2
1:A:71:ILE:HD12	1:A:76:LYS:HD3	0.54	1.79	13	1
1:A:75:ALA:HB3	1:A:77:GLN:HE22	0.54	1.62	12	1
1:A:52:THR:HG23	1:A:156:GLN:HB3	0.54	1.79	9	1
1:A:51:ALA:HB2	1:A:73:PHE:CE2	0.53	2.38	18	2
1:A:71:ILE:C	1:A:71:ILE:HD12	0.53	2.29	30	5
1:A:77:GLN:NE2	1:A:77:GLN:H	0.53	2.01	13	2
1:A:51:ALA:HB2	1:A:71:ILE:CG1	0.52	2.35	26	2
1:A:51:ALA:HB3	1:A:71:ILE:HG13	0.52	1.80	1	6
1:A:119:GLU:CD	1:A:141:VAL:HG21	0.52	2.29	28	1
1:A:51:ALA:HB3	1:A:71:ILE:CG1	0.51	2.35	24	4
1:A:71:ILE:HG22	1:A:78:GLY:CA	0.50	2.37	13	1
1:A:53:TYR:CE1	1:A:71:ILE:HG21	0.50	2.41	3	2
1:A:123:TYR:CD1	1:A:139:ALA:HB2	0.49	2.42	1	1
1:A:109:ILE:HD12	1:A:110:SER:N	0.48	2.23	22	2
1:A:83:GLU:C	1:A:84:HIS:CG	0.48	2.91	13	2
1:A:66:LYS:HE2	1:A:84:HIS:CG	0.47	2.43	13	2
1:A:125:LEU:HD23	1:A:152:LEU:HD12	0.47	1.85	22	6
1:A:139:ALA:HB3	1:A:150:ILE:HB	0.47	1.87	8	1
1:A:45:LEU:HD11	1:A:127:ILE:HD12	0.47	1.85	13	1
1:A:61:ASP:OD2	1:A:86:LYS:NZ	0.46	2.49	2	2
1:A:82:ILE:O	1:A:82:ILE:HG22	0.46	2.10	21	3
1:A:83:GLU:O	1:A:84:HIS:CD2	0.46	2.68	11	1
1:A:139:ALA:HB1	1:A:141:VAL:HG13	0.46	1.87	6	1
1:A:71:ILE:HD11	1:A:73:PHE:CD1	0.45	2.46	3	1
1:A:80:GLY:O	1:A:94:LEU:HD12	0.45	2.11	16	1
1:A:51:ALA:HB1	1:A:53:TYR:CE1	0.45	2.46	26	1
1:A:71:ILE:CG2	1:A:78:GLY:HA2	0.45	2.42	18	2
1:A:53:TYR:CE1	1:A:71:ILE:CG2	0.44	3.00	3	1
1:A:92:VAL:HG22	1:A:115:TYR:HA	0.44	1.88	2	1
1:A:125:LEU:HD21	1:A:135:VAL:HB	0.44	1.89	26	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:HIS:CD2	1:A:127:ILE:H	0.44	2.30	17	1
1:A:42:PHE:C	1:A:42:PHE:CD2	0.44	2.94	24	1
1:A:71:ILE:HD12	1:A:76:LYS:CD	0.44	2.41	13	1
1:A:101:PRO:O	1:A:102:ASP:CB	0.44	2.66	6	1
1:A:127:ILE:HA	1:A:135:VAL:HG12	0.43	1.89	5	1
1:A:94:LEU:HD13	1:A:123:TYR:CE2	0.43	2.49	14	1
1:A:40:THR:HG23	1:A:106:HIS:HB2	0.43	1.89	7	1
1:A:39:HIS:CB	1:A:106:HIS:HA	0.43	2.44	20	1
1:A:65:GLY:CA	1:A:82:ILE:HG23	0.43	2.41	23	1
1:A:77:GLN:H	1:A:77:GLN:CD	0.42	2.21	13	1
1:A:141:VAL:O	1:A:141:VAL:HG23	0.42	2.13	10	1
1:A:120:LYS:N	1:A:120:LYS:CD	0.42	2.83	23	1
1:A:127:ILE:C	1:A:127:ILE:HD13	0.42	2.39	26	1
1:A:81:LYS:NZ	1:A:83:GLU:OE1	0.42	2.51	11	1
1:A:120:LYS:N	1:A:120:LYS:HD3	0.42	2.29	23	1
1:A:53:TYR:CE1	1:A:135:VAL:HG13	0.42	2.50	5	1
1:A:51:ALA:HB1	1:A:53:TYR:CD1	0.41	2.50	29	1
1:A:102:ASP:OD1	1:A:104:LYS:NZ	0.41	2.53	27	1
1:A:71:ILE:HD12	1:A:76:LYS:HG3	0.41	1.93	17	1
1:A:106:HIS:CD2	1:A:127:ILE:HG22	0.41	2.50	17	1
1:A:89:GLU:N	1:A:89:GLU:CD	0.41	2.79	18	1
1:A:38:GLU:OE1	1:A:100:LYS:NZ	0.41	2.54	22	1
1:A:53:TYR:CD1	1:A:71:ILE:HG21	0.41	2.50	24	1
1:A:141:VAL:HG22	1:A:142:LYS:N	0.41	2.26	28	1
1:A:134:GLU:OE1	1:A:155:LYS:NZ	0.41	2.53	16	1
1:A:42:PHE:CD1	1:A:42:PHE:C	0.41	2.99	19	1
1:A:155:LYS:NZ	1:A:156:GLN:O	0.41	2.53	11	1
1:A:134:GLU:OE2	1:A:155:LYS:NZ	0.41	2.53	17	1
1:A:120:LYS:HA	1:A:120:LYS:CE	0.41	2.46	11	1
1:A:102:ASP:OD2	1:A:104:LYS:NZ	0.41	2.53	22	1
1:A:143:THR:HG23	1:A:145:ASN:H	0.41	1.75	27	1
1:A:76:LYS:H	1:A:77:GLN:NE2	0.40	2.15	19	1
1:A:71:ILE:HD13	1:A:76:LYS:HG2	0.40	1.93	30	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	119/164 (73%)	87±4 (73±3%)	25±4 (21±3%)	7±2 (6±2%)	2	20
All	All	3570/4920 (73%)	2615 (73%)	743 (21%)	212 (6%)	2	20

All 38 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	44	LYS	26
1	A	38	GLU	21
1	A	62	ASP	15
1	A	132	ALA	12
1	A	106	HIS	12
1	A	100	LYS	12
1	A	76	LYS	11
1	A	148	ARG	10
1	A	102	ASP	7
1	A	116	ASN	7
1	A	130	GLY	7
1	A	104	LYS	7
1	A	105	ARG	7
1	A	46	PRO	7
1	A	103	GLY	5
1	A	107	ALA	5
1	A	84	HIS	4
1	A	37	GLY	4
1	A	48	GLY	3
1	A	90	LEU	3
1	A	131	LYS	3
1	A	40	THR	2
1	A	73	PHE	2
1	A	101	PRO	2
1	A	49	GLY	2
1	A	78	GLY	2
1	A	91	ASN	2
1	A	129	GLY	2
1	A	74	ALA	1
1	A	43	ASP	1
1	A	47	GLU	1
1	A	149	HIS	1
1	A	85	LEU	1
1	A	99	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	86	LYS	1
1	A	45	LEU	1
1	A	79	ASN	1
1	A	142	LYS	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	87/125 (70%)	69±3 (80±4%)	18±3 (20±4%)	3	32
All	All	2610/3750 (70%)	2077 (80%)	533 (20%)	3	32

All 65 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	86	LYS	30
1	A	113	VAL	28
1	A	71	ILE	27
1	A	147	ILE	24
1	A	99	ILE	23
1	A	127	ILE	21
1	A	77	GLN	18
1	A	152	LEU	18
1	A	50	ARG	15
1	A	66	LYS	15
1	A	125	LEU	15
1	A	94	LEU	14
1	A	114	LEU	14
1	A	123	TYR	14
1	A	76	LYS	12
1	A	142	LYS	12
1	A	81	LYS	11
1	A	44	LYS	11
1	A	104	LYS	11
1	A	145	ASN	11
1	A	79	ASN	9

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Mol	Chain	Res	Type	Models (Total)
1	A	117	GLN	9
1	A	89	GLU	9
1	A	100	LYS	9
1	A	41	SER	8
1	A	122	SER	8
1	A	90	LEU	8
1	A	155	LYS	8
1	A	115	TYR	8
1	A	120	LYS	8
1	A	135	VAL	7
1	A	38	GLU	6
1	A	102	ASP	6
1	A	68	THR	6
1	A	156	GLN	6
1	A	87	SER	6
1	A	43	ASP	5
1	A	93	ASP	5
1	A	108	VAL	5
1	A	84	HIS	4
1	A	109	ILE	4
1	A	39	HIS	4
1	A	82	ILE	4
1	A	70	THR	3
1	A	150	ILE	3
1	A	91	ASN	2
1	A	54	ARG	2
1	A	143	THR	2
1	A	133	GLN	2
1	A	40	THR	2
1	A	60	SER	2
1	A	52	THR	2
1	A	47	GLU	2
1	A	105	ARG	2
1	A	42	PHE	2
1	A	131	LYS	2
1	A	140	GLU	1
1	A	148	ARG	1
1	A	45	LEU	1
1	A	62	ASP	1
1	A	83	GLU	1
1	A	98	ASP	1
1	A	106	HIS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	119	GLU	1
1	A	58	PHE	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

No chemical shift data were provided