



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 07:44 PM UTC

PDB ID : 2KC0 / pdb_00002kc0
Title : Solution structure of the factor H binding protein
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Deposited on : 2008-12-13

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

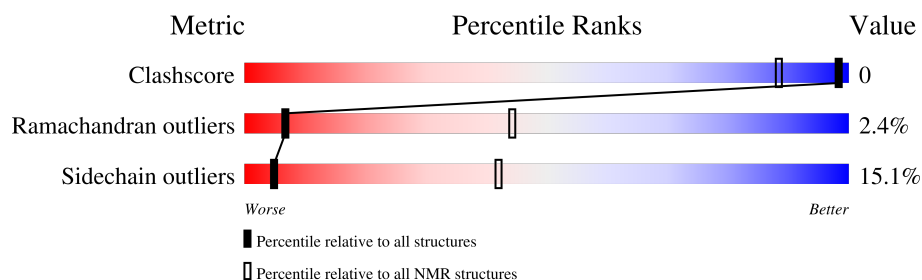
1 Overall quality at a glance

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	255	

2 Ensemble composition and analysis ⓘ

This entry contains 25 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:14-A:24, (236) A:31-A:255	1.44	4

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 4 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3648 atoms, of which 1820 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called lipoprotein.

Mol	Chain	Residues	Atoms						Trace
1	A	242	Total	C	H	N	O	S	0
			3648	1135	1820	329	363	1	

There are 7 discrepancies between the modelled and reference sequences:

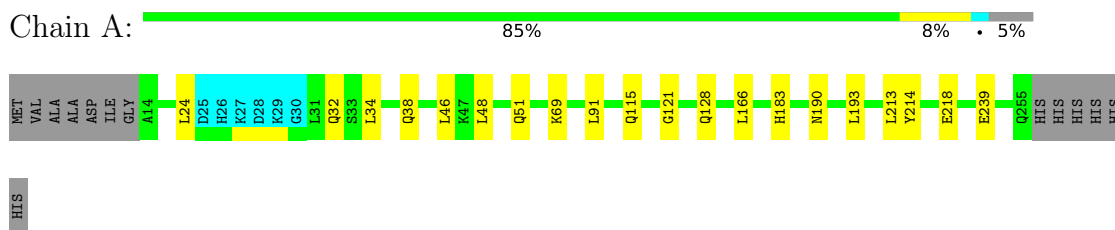
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	expression tag	UNP Q6VRZ6
A	256	HIS	-	expression tag	UNP Q6VRZ6
A	257	HIS	-	expression tag	UNP Q6VRZ6
A	258	HIS	-	expression tag	UNP Q6VRZ6
A	259	HIS	-	expression tag	UNP Q6VRZ6
A	260	HIS	-	expression tag	UNP Q6VRZ6
A	261	HIS	-	expression tag	UNP Q6VRZ6

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

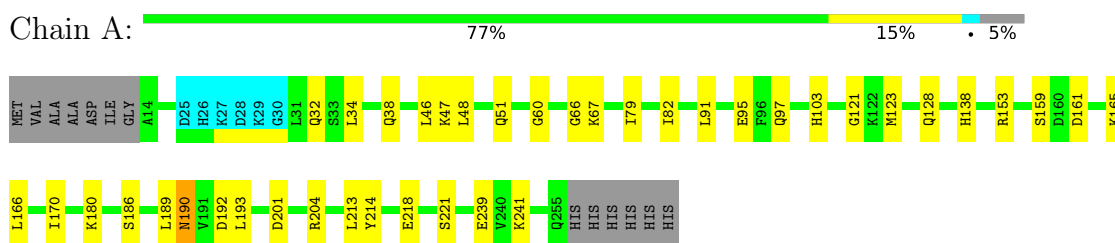


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

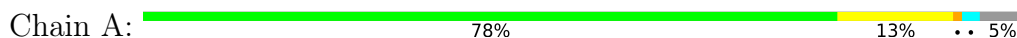
4.2.1 Score per residue for model 1

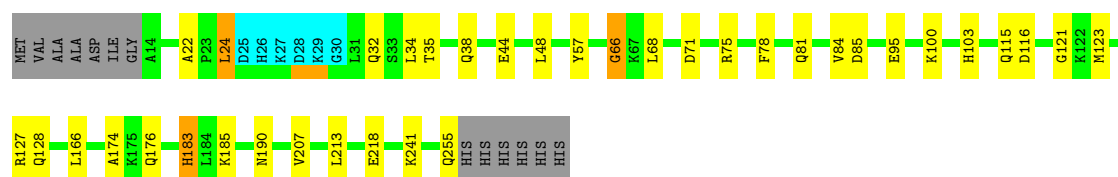
- Molecule 1: lipoprotein



4.2.2 Score per residue for model 2

- Molecule 1: lipoprotein





4.2.3 Score per residue for model 3

- Molecule 1: lipoprotein

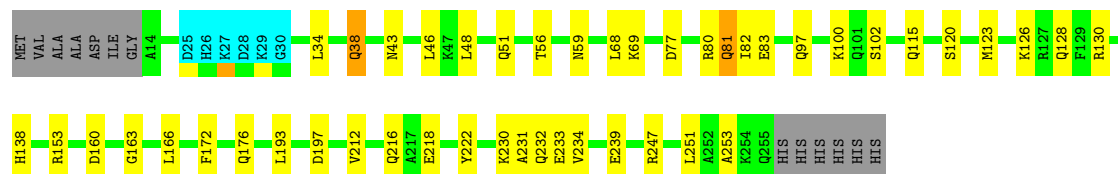
Chain A: 80% 12% 5%



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: lipoprotein

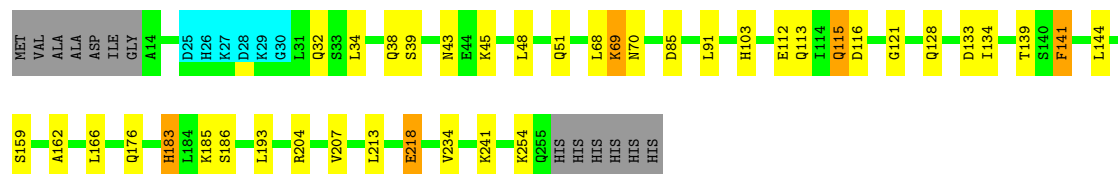
Chain A: 75% 17% 5%



4.2.5 Score per residue for model 5

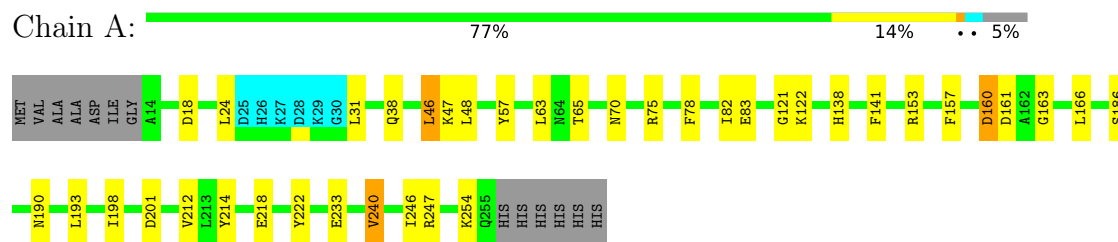
- Molecule 1: lipoprotein

Chain A: 77% 14% 5%



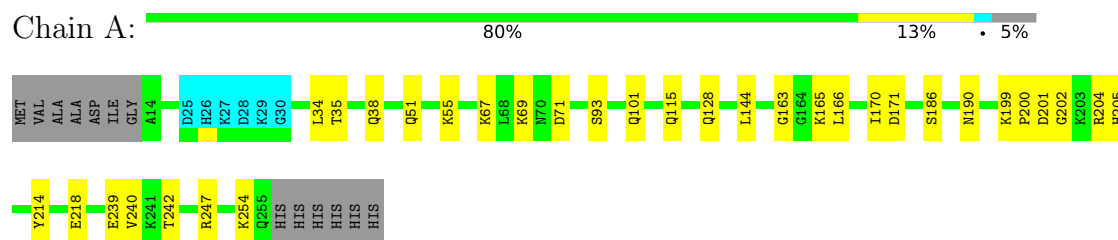
4.2.6 Score per residue for model 6

- Molecule 1: lipoprotein



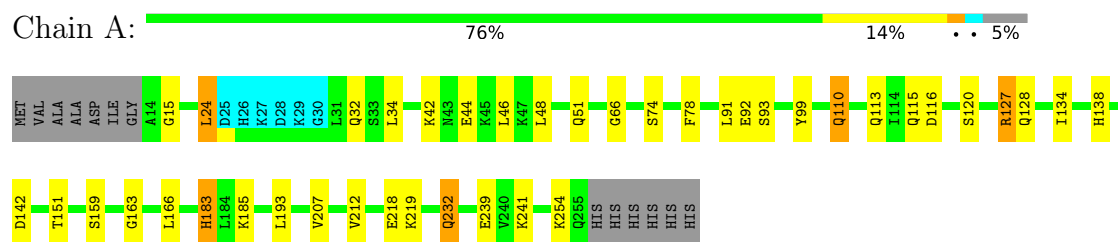
4.2.7 Score per residue for model 7

- Molecule 1: lipoprotein



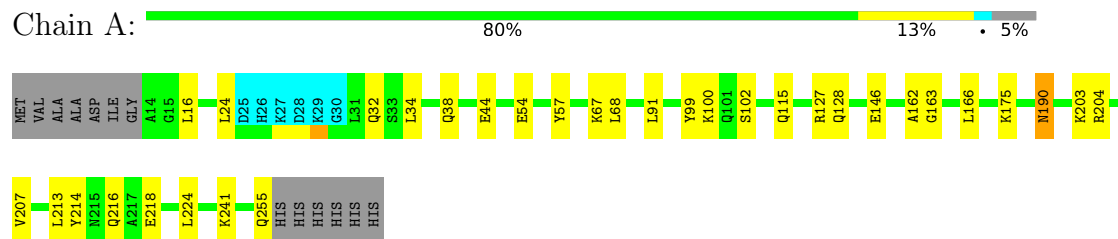
4.2.8 Score per residue for model 8

- Molecule 1: lipoprotein



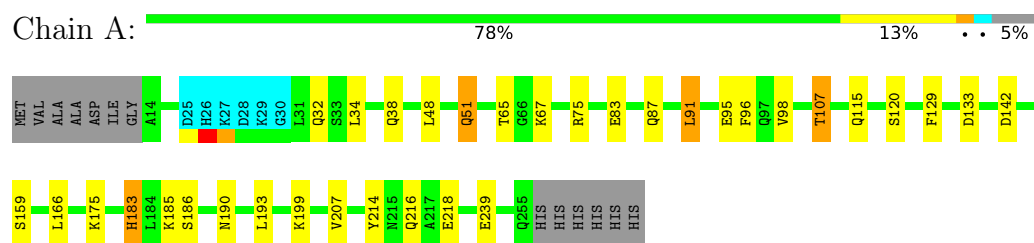
4.2.9 Score per residue for model 9

- Molecule 1: lipoprotein



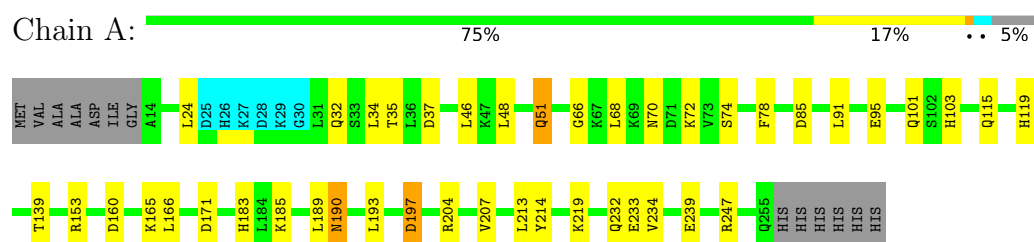
4.2.10 Score per residue for model 10

- Molecule 1: lipoprotein



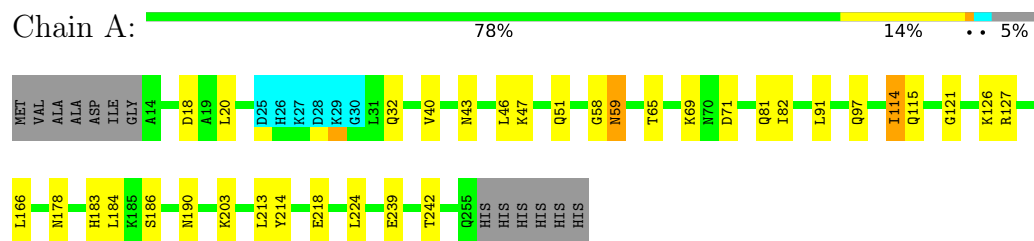
4.2.11 Score per residue for model 11

- Molecule 1: lipoprotein



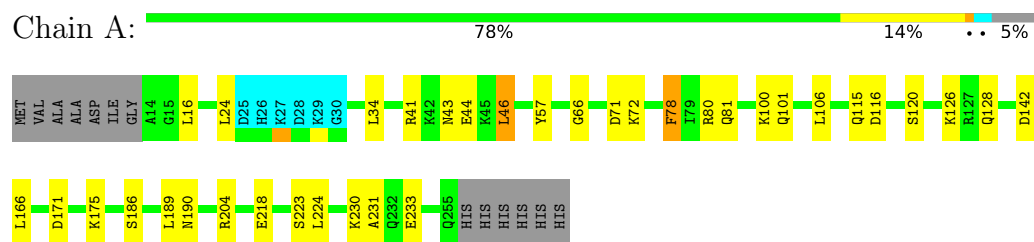
4.2.12 Score per residue for model 12

- Molecule 1: lipoprotein



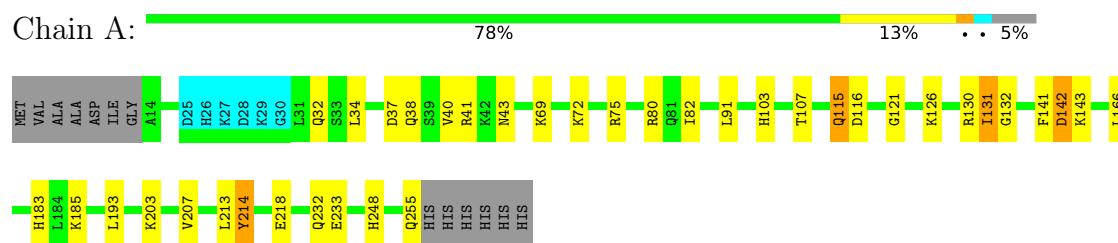
4.2.13 Score per residue for model 13

- Molecule 1: lipoprotein



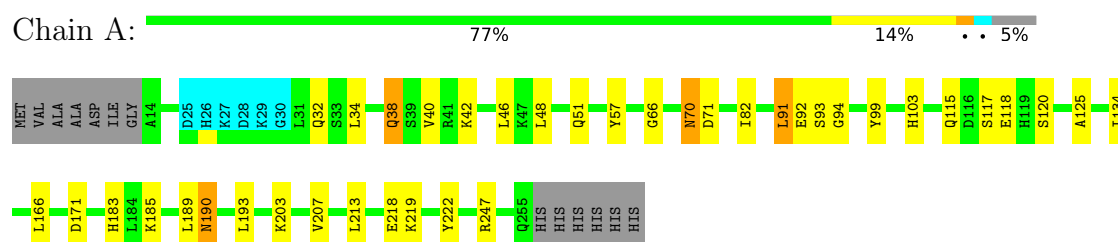
4.2.14 Score per residue for model 14

- Molecule 1: lipoprotein



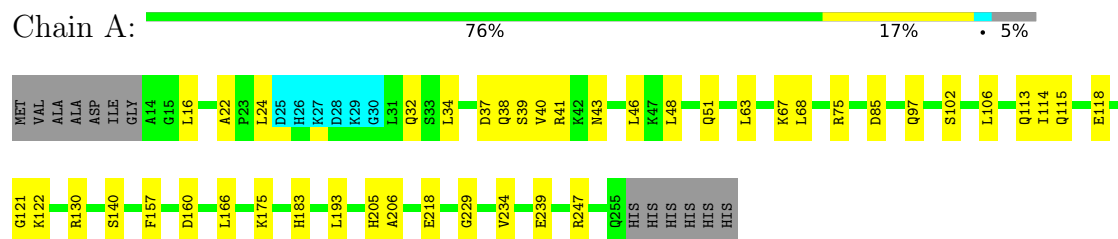
4.2.15 Score per residue for model 15

- Molecule 1: lipoprotein



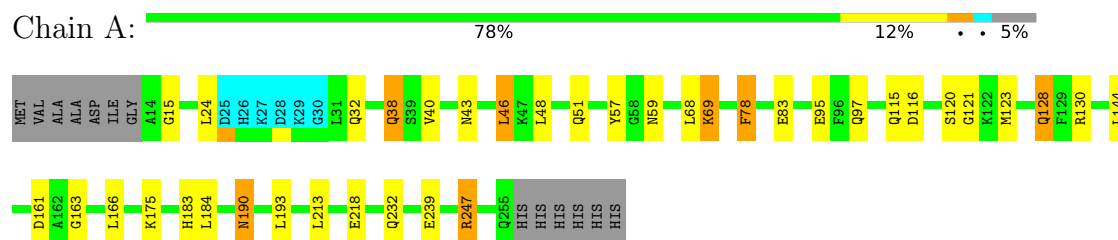
4.2.16 Score per residue for model 16

- Molecule 1: lipoprotein



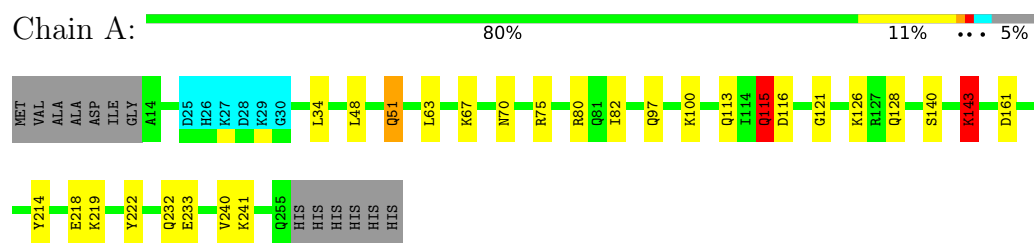
4.2.17 Score per residue for model 17

- Molecule 1: lipoprotein



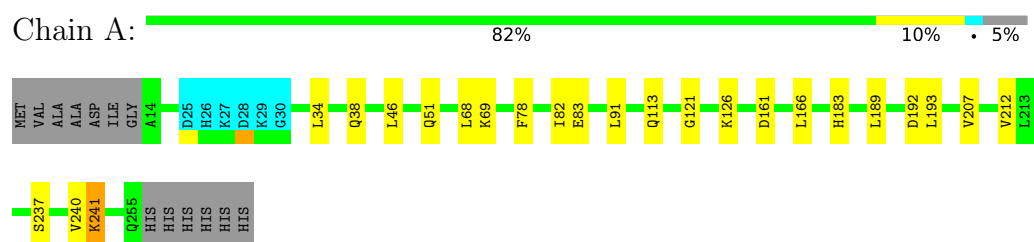
4.2.18 Score per residue for model 18

- Molecule 1: lipoprotein



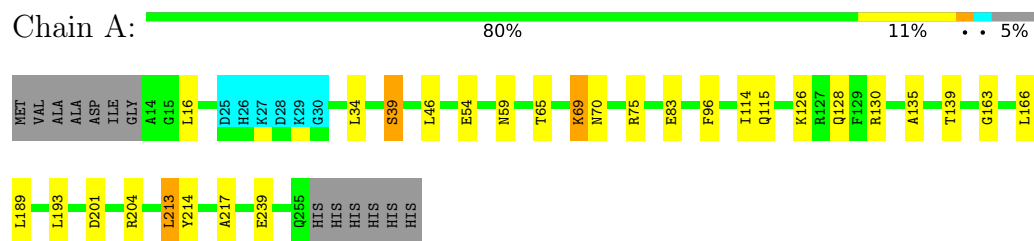
4.2.19 Score per residue for model 19

- Molecule 1: lipoprotein



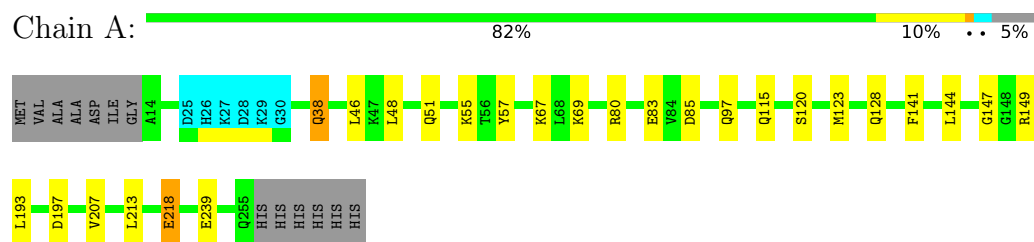
4.2.20 Score per residue for model 20

- Molecule 1: lipoprotein



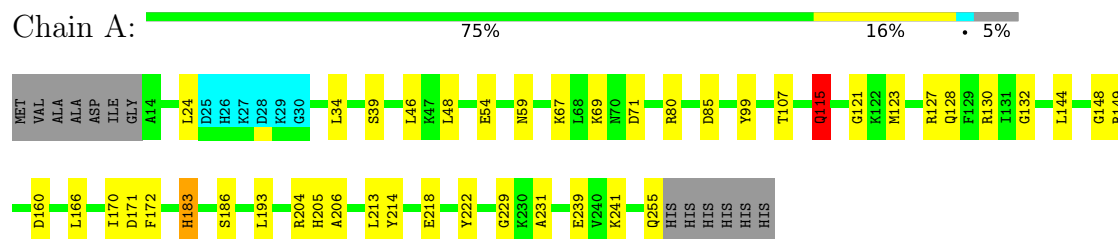
4.2.21 Score per residue for model 21

- Molecule 1: lipoprotein



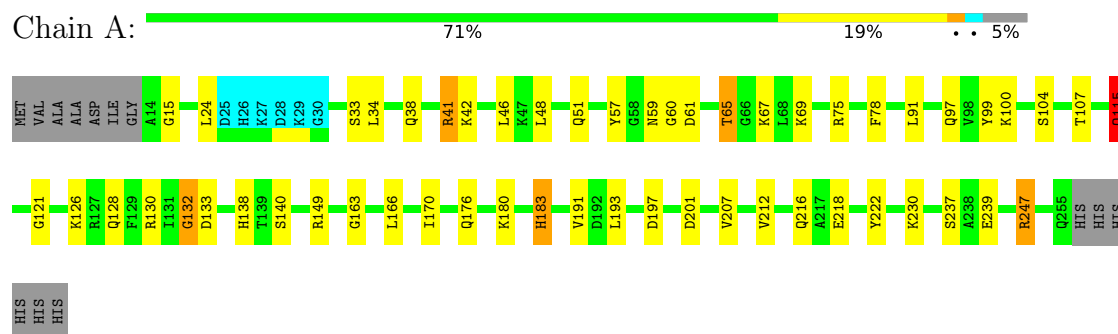
4.2.22 Score per residue for model 22

- Molecule 1: lipoprotein



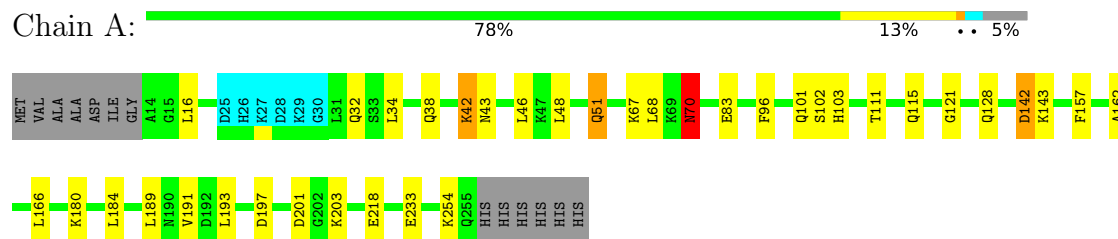
4.2.23 Score per residue for model 23

- Molecule 1: lipoprotein



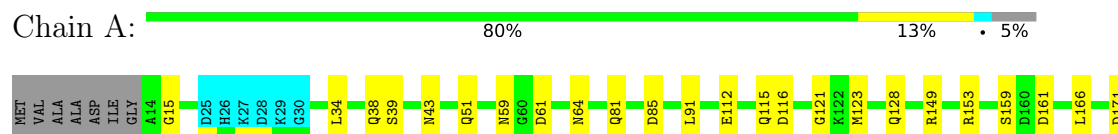
4.2.24 Score per residue for model 24

- Molecule 1: lipoprotein



4.2.25 Score per residue for model 25

- Molecule 1: lipoprotein



K175	H183	L184	K185	S186	L189	L193	L213	Y214	K230	Q265	HIS	HIS	HIS	HIS	HIS	HIS
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5 Refinement protocol and experimental data overview

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

Of the 900 calculated structures, 25 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	
CYANA	refinement	

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	0.89±0.01	0±0/1804 (0.0± 0.0%)	1.48±0.03	6±3/2422 (0.3± 0.1%)
All	All	0.89	0/45100 (0.0%)	1.48	158/60550 (0.3%)

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	1.1±0.9
All	All	0	28

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	172	PHE	CA-CB-CG	8.43	122.23	113.80	4	1
1	A	190	ASN	CA-CB-CG	7.94	120.54	112.60	3	10
1	A	163	GLY	CA-C-N	7.92	127.52	119.92	23	5
1	A	163	GLY	C-N-CA	7.92	127.52	119.92	23	5
1	A	197	ASP	CA-CB-CG	7.91	120.51	112.60	11	4
1	A	116	ASP	CA-CB-CG	7.78	120.38	112.60	5	1
1	A	32	GLN	OE1-CD-NE2	-7.57	115.03	122.60	2	4
1	A	160	ASP	CA-CB-CG	7.45	120.05	112.60	6	1
1	A	96	PHE	CA-CB-CG	7.05	120.85	113.80	20	2
1	A	71	ASP	CA-CB-CG	6.74	119.34	112.60	13	2
1	A	115	GLN	N-CA-CB	-6.58	101.04	110.44	14	4
1	A	69	LYS	CA-C-N	6.46	133.88	121.54	5	1
1	A	69	LYS	C-N-CA	6.46	133.88	121.54	5	1
1	A	247	ARG	CD-NE-CZ	6.44	133.41	124.40	23	1
1	A	18	ASP	CA-CB-CG	6.35	118.95	112.60	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	132	GLY	CA-C-N	6.29	133.56	121.54	23	1
1	A	132	GLY	C-N-CA	6.29	133.56	121.54	23	1
1	A	142	ASP	CA-C-N	6.29	129.86	120.17	24	5
1	A	142	ASP	C-N-CA	6.29	129.86	120.17	24	5
1	A	229	GLY	CA-C-N	6.28	129.89	119.35	16	1
1	A	229	GLY	C-N-CA	6.28	129.89	119.35	16	1
1	A	125	ALA	N-CA-C	6.21	119.35	110.10	15	1
1	A	70	ASN	CA-CB-CG	6.15	118.75	112.60	24	1
1	A	78	PHE	CA-CB-CG	6.14	119.94	113.80	17	6
1	A	218	GLU	N-CA-C	5.98	117.61	110.19	2	1
1	A	115	GLN	CB-CA-C	5.94	122.69	110.40	24	6
1	A	24	LEU	CA-C-N	5.94	132.77	122.32	22	1
1	A	24	LEU	C-N-CA	5.94	132.77	122.32	22	1
1	A	203	LYS	N-CA-C	5.89	120.00	112.34	15	2
1	A	38	GLN	CA-C-N	5.87	128.41	120.38	15	4
1	A	38	GLN	C-N-CA	5.87	128.41	120.38	15	4
1	A	68	LEU	N-CA-C	5.80	120.42	113.23	2	1
1	A	78	PHE	N-CA-C	5.78	117.96	109.24	2	1
1	A	93	SER	N-CA-C	5.77	118.05	108.99	15	1
1	A	141	PHE	CA-CB-CG	5.76	119.56	113.80	5	3
1	A	43	ASN	CA-CB-CG	5.72	118.32	112.60	24	2
1	A	129	PHE	CA-CB-CG	5.67	119.47	113.80	10	1
1	A	184	LEU	CA-C-N	5.64	129.62	120.60	25	2
1	A	184	LEU	C-N-CA	5.64	129.62	120.60	25	2
1	A	114	ILE	CA-C-N	5.63	128.83	120.95	12	1
1	A	114	ILE	C-N-CA	5.63	128.83	120.95	12	1
1	A	214	TYR	N-CA-C	5.61	117.66	108.52	14	1
1	A	170	ILE	CB-CA-C	5.59	116.78	110.41	7	1
1	A	126	LYS	N-CA-C	5.53	119.19	111.56	4	1
1	A	41	ARG	CA-C-N	5.51	128.43	120.38	16	1
1	A	41	ARG	C-N-CA	5.51	128.43	120.38	16	1
1	A	128	GLN	N-CA-C	5.49	117.25	108.41	17	1
1	A	115	GLN	N-CA-C	5.48	116.98	110.19	21	1
1	A	72	LYS	N-CA-C	5.42	117.43	109.24	13	1
1	A	115	GLN	CB-CG-CD	-5.42	103.38	112.60	20	1
1	A	190	ASN	OD1-CG-ND2	-5.40	117.20	122.60	3	6
1	A	166	LEU	N-CA-C	5.39	117.18	109.14	18	1
1	A	174	ALA	CA-C-N	5.38	129.81	122.34	2	1
1	A	174	ALA	C-N-CA	5.38	129.81	122.34	2	1
1	A	66	GLY	CA-C-N	5.37	127.80	120.54	11	1
1	A	66	GLY	C-N-CA	5.37	127.80	120.54	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	67	LYS	CA-C-N	5.34	127.87	120.29	18	1
1	A	67	LYS	C-N-CA	5.34	127.87	120.29	18	1
1	A	51	GLN	OE1-CD-NE2	-5.28	117.32	122.60	10	4
1	A	61	ASP	N-CA-C	5.27	115.24	108.34	23	1
1	A	138	HIS	CB-CG-CD2	-5.26	124.36	131.20	4	1
1	A	232	GLN	OE1-CD-NE2	-5.25	117.35	122.60	18	2
1	A	139	THR	CA-C-N	5.22	128.28	120.87	11	1
1	A	139	THR	C-N-CA	5.22	128.28	120.87	11	1
1	A	44	GLU	N-CA-CB	-5.19	102.46	110.56	13	1
1	A	157	PHE	CA-CB-CG	5.19	118.99	113.80	6	1
1	A	157	PHE	CA-C-N	5.18	128.65	121.09	24	1
1	A	157	PHE	C-N-CA	5.18	128.65	121.09	24	1
1	A	59	ASN	CA-CB-CG	5.17	117.77	112.60	12	1
1	A	94	GLY	N-CA-C	5.17	118.68	111.19	15	1
1	A	171	ASP	CA-C-N	5.17	127.46	120.38	11	2
1	A	171	ASP	C-N-CA	5.17	127.46	120.38	11	2
1	A	143	LYS	CA-CB-CG	5.15	124.41	114.10	18	1
1	A	191	VAL	N-CA-C	5.13	116.69	108.89	24	1
1	A	135	ALA	CA-C-N	5.13	126.77	120.51	20	1
1	A	135	ALA	C-N-CA	5.13	126.77	120.51	20	1
1	A	178	ASN	N-CA-CB	-5.07	103.22	110.87	12	1
1	A	81	GLN	OE1-CD-NE2	-5.06	117.54	122.60	4	1
1	A	65	THR	CA-C-N	5.06	126.50	120.13	6	1
1	A	65	THR	C-N-CA	5.06	126.50	120.13	6	1
1	A	170	ILE	N-CA-C	5.06	115.32	107.78	22	1
1	A	198	ILE	N-CA-C	5.06	116.10	109.58	6	1
1	A	133	ASP	CA-CB-CG	5.04	117.64	112.60	10	1
1	A	255	GLN	OE1-CD-NE2	-5.01	117.59	122.60	22	1
1	A	158	GLY	CA-C-N	5.01	131.10	121.54	10	1
1	A	158	GLY	C-N-CA	5.01	131.10	121.54	10	1
1	A	110	GLN	OE1-CD-NE2	-5.00	117.59	122.60	8	1
1	A	183	HIS	CB-CG-CD2	-5.00	124.70	131.20	11	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	57	TYR	Sidechain	8
1	A	127	ARG	Sidechain	3
1	A	222	TYR	Sidechain	3

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	41	ARG	Sidechain	3
1	A	80	ARG	Sidechain	3
1	A	149	ARG	Sidechain	2
1	A	247	ARG	Sidechain	2
1	A	214	TYR	Sidechain	1
1	A	130	ARG	Sidechain	1
1	A	115	GLN	Sidechain	1
1	A	75	ARG	Sidechain	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	1780	1776	1775	1±1
All	All	44500	44400	44375	29

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:LEU:HD13	1:A:78:PHE:CZ	0.72	2.18	17	2
1:A:46:LEU:HD13	1:A:78:PHE:CE2	0.69	2.22	13	2
1:A:96:PHE:CE1	1:A:107:THR:HG21	0.67	2.24	10	1
1:A:96:PHE:CZ	1:A:107:THR:HG21	0.60	2.31	10	1
1:A:214:TYR:CD1	1:A:240:VAL:HG21	0.54	2.37	19	2
1:A:115:GLN:HE21	1:A:116:ASP:N	0.51	2.04	18	1
1:A:115:GLN:HE21	1:A:115:GLN:C	0.49	2.15	18	1
1:A:24:LEU:H	1:A:24:LEU:HD23	0.48	1.68	9	1
1:A:103:HIS:CD2	1:A:232:GLN:NE2	0.47	2.82	14	2
1:A:91:LEU:HD13	1:A:91:LEU:H	0.46	1.71	15	1
1:A:214:TYR:CE1	1:A:240:VAL:HG11	0.46	2.45	7	1
1:A:240:VAL:HG22	1:A:241:LYS:O	0.45	2.11	19	1
1:A:193:LEU:HD21	1:A:222:TYR:CE1	0.44	2.47	3	1
1:A:106:LEU:HD11	1:A:157:PHE:CZ	0.44	2.47	16	2
1:A:115:GLN:C	1:A:115:GLN:HE21	0.44	2.20	22	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:LEU:HD11	1:A:78:PHE:CE2	0.43	2.48	6	1
1:A:213:LEU:CD1	1:A:217:ALA:N	0.43	2.82	20	1
1:A:24:LEU:HD23	1:A:66:GLY:H	0.42	1.74	2	1
1:A:69:LYS:CG	1:A:70:ASN:H	0.42	2.27	20	1
1:A:141:PHE:C	1:A:143:LYS:H	0.41	2.24	14	1
1:A:131:ILE:HD13	1:A:131:ILE:C	0.41	2.41	14	1
1:A:38:GLN:H	1:A:38:GLN:NE2	0.40	2.14	17	1
1:A:214:TYR:CE1	1:A:240:VAL:HG21	0.40	2.50	6	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	234/255 (92%)	201±4 (86±2%)	28±4 (12±2%)	6±2 (2±1%)	7	44
All	All	5850/6375 (92%)	5019 (86%)	690 (12%)	141 (2%)	7	44

All 49 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	121	GLY	14
1	A	183	HIS	13
1	A	120	SER	6
1	A	70	ASN	6
1	A	66	GLY	5
1	A	59	ASN	5
1	A	68	LEU	5
1	A	161	ASP	4
1	A	159	SER	4
1	A	15	GLY	4
1	A	127	ARG	4
1	A	60	GLY	3
1	A	103	HIS	3
1	A	204	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	A	24	LEU	3
1	A	67	LYS	3
1	A	163	GLY	3
1	A	231	ALA	3
1	A	162	ALA	3
1	A	102	SER	3
1	A	65	THR	3
1	A	132	GLY	3
1	A	42	LYS	3
1	A	39	SER	3
1	A	201	ASP	2
1	A	22	ALA	2
1	A	160	ASP	2
1	A	230	LYS	2
1	A	218	GLU	2
1	A	206	ALA	2
1	A	69	LYS	2
1	A	203	LYS	1
1	A	253	ALA	1
1	A	144	LEU	1
1	A	200	PRO	1
1	A	202	GLY	1
1	A	91	LEU	1
1	A	58	GLY	1
1	A	142	ASP	1
1	A	117	SER	1
1	A	118	GLU	1
1	A	122	LYS	1
1	A	143	LYS	1
1	A	147	GLY	1
1	A	71	ASP	1
1	A	148	GLY	1
1	A	229	GLY	1
1	A	133	ASP	1
1	A	180	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	183/198 (92%)	155±5 (85±3%)	28±5 (15±3%)	5	42
All	All	4575/4950 (92%)	3884 (85%)	691 (15%)	5	42

All 142 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	166	LEU	25
1	A	34	LEU	21
1	A	218	GLU	21
1	A	193	LEU	19
1	A	51	GLN	18
1	A	128	GLN	18
1	A	115	GLN	18
1	A	38	GLN	17
1	A	48	LEU	17
1	A	46	LEU	16
1	A	91	LEU	13
1	A	213	LEU	13
1	A	239	GLU	13
1	A	183	HIS	11
1	A	207	VAL	11
1	A	69	LYS	11
1	A	189	LEU	10
1	A	186	SER	9
1	A	82	ILE	8
1	A	97	GLN	8
1	A	241	LYS	8
1	A	185	LYS	8
1	A	32	GLN	8
1	A	247	ARG	8
1	A	83	GLU	8
1	A	233	GLU	8
1	A	214	TYR	8
1	A	67	LYS	7
1	A	123	MET	7
1	A	153	ARG	7
1	A	75	ARG	7
1	A	85	ASP	7
1	A	100	LYS	7
1	A	24	LEU	7
1	A	43	ASN	7
1	A	175	LYS	7

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Mol	Chain	Res	Type	Models (Total)
1	A	126	LYS	7
1	A	190	ASN	6
1	A	116	ASP	6
1	A	113	GLN	6
1	A	130	ARG	6
1	A	95	GLU	5
1	A	81	GLN	5
1	A	176	GLN	5
1	A	101	GLN	5
1	A	212	VAL	5
1	A	204	ARG	5
1	A	254	LYS	5
1	A	144	LEU	5
1	A	99	TYR	5
1	A	16	LEU	5
1	A	40	VAL	5
1	A	138	HIS	4
1	A	161	ASP	4
1	A	165	LYS	4
1	A	54	GLU	4
1	A	160	ASP	4
1	A	216	GLN	4
1	A	222	TYR	4
1	A	234	VAL	4
1	A	201	ASP	4
1	A	219	LYS	4
1	A	107	THR	4
1	A	171	ASP	4
1	A	47	LYS	3
1	A	35	THR	3
1	A	44	GLU	3
1	A	71	ASP	3
1	A	255	GLN	3
1	A	133	ASP	3
1	A	80	ARG	3
1	A	232	GLN	3
1	A	39	SER	3
1	A	68	LEU	3
1	A	134	ILE	3
1	A	63	LEU	3
1	A	205	HIS	3
1	A	142	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	203	LYS	3
1	A	224	LEU	3
1	A	37	ASP	3
1	A	114	ILE	3
1	A	140	SER	3
1	A	149	ARG	3
1	A	170	ILE	2
1	A	180	LYS	2
1	A	192	ASP	2
1	A	103	HIS	2
1	A	61	ASP	2
1	A	197	ASP	2
1	A	112	GLU	2
1	A	139	THR	2
1	A	55	LYS	2
1	A	93	SER	2
1	A	199	LYS	2
1	A	242	THR	2
1	A	42	LYS	2
1	A	74	SER	2
1	A	92	GLU	2
1	A	65	THR	2
1	A	72	LYS	2
1	A	59	ASN	2
1	A	184	LEU	2
1	A	70	ASN	2
1	A	143	LYS	2
1	A	237	SER	2
1	A	230	LYS	2
1	A	79	ILE	1
1	A	159	SER	1
1	A	221	SER	1
1	A	84	VAL	1
1	A	198	ILE	1
1	A	56	THR	1
1	A	77	ASP	1
1	A	102	SER	1
1	A	251	LEU	1
1	A	45	LYS	1
1	A	141	PHE	1
1	A	31	LEU	1
1	A	122	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	240	VAL	1
1	A	246	ILE	1
1	A	110	GLN	1
1	A	151	THR	1
1	A	146	GLU	1
1	A	87	GLN	1
1	A	98	VAL	1
1	A	119	HIS	1
1	A	18	ASP	1
1	A	20	LEU	1
1	A	223	SER	1
1	A	131	ILE	1
1	A	248	HIS	1
1	A	118	GLU	1
1	A	120	SER	1
1	A	172	PHE	1
1	A	33	SER	1
1	A	41	ARG	1
1	A	104	SER	1
1	A	191	VAL	1
1	A	111	THR	1
1	A	64	ASN	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