Full wwPDB NMR Structure Validation Report (i)

Jun 22, 2024 – 09:59 PM EDT

PDB ID	:	6D5Z
Title	:	Cis form of Hemolysin II C-terminal domain
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Deposited on	:	2018-04-19

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 (i) 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 (i)) were used in the production of this report:

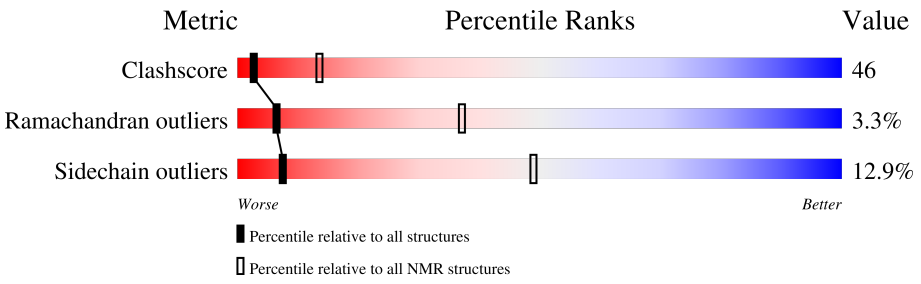
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	D	98	27% 50% 7% 12% •

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 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	D:13-D:94 (82)	0.65	3

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. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1460 atoms, of which 728 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hemolysin II.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	D	94	1460	454	728	126	150	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP Q81AN8
D	-2	SER	-	expression tag	UNP Q81AN8
D	-1	HIS	-	expression tag	UNP Q81AN8
D	0	MET	-	expression tag	UNP Q81AN8

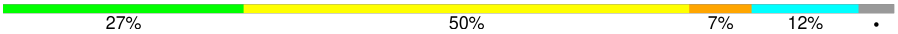
4 Residue-property plots (i)

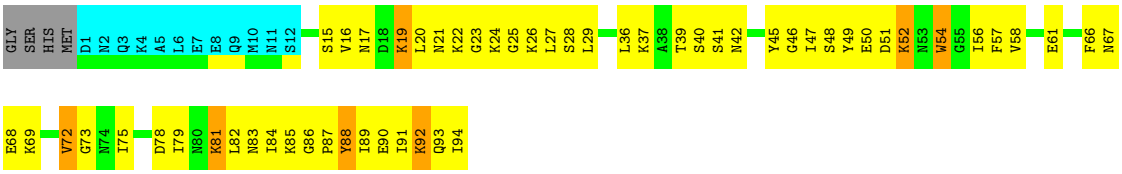
4.1 Average score per residue in the NMR ensemble

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: Hemolysin II

Chain D:





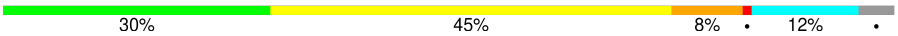
4.2 Scores per residue for each member of the ensemble

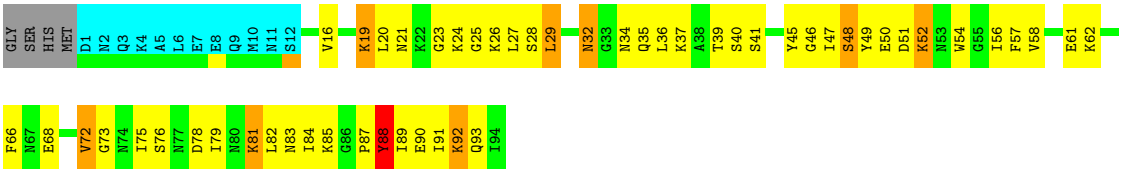
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Hemolysin II

Chain D:

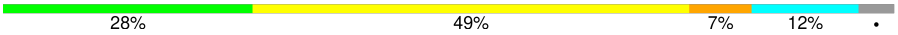


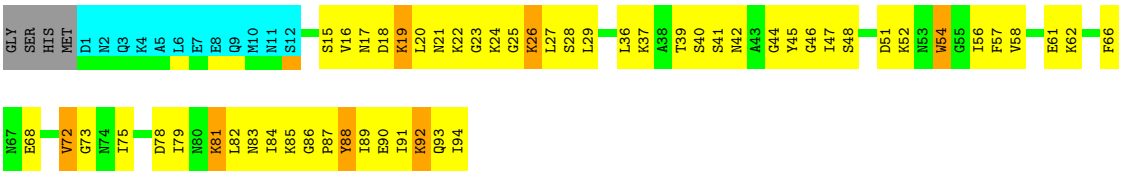


4.2.2 Score per residue for model 2

• Molecule 1: Hemolysin II

Chain D:

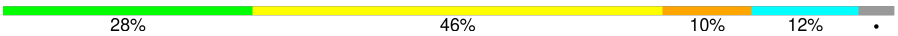


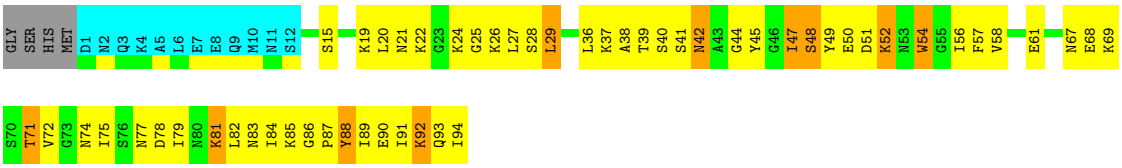


4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Hemolysin II

Chain D:

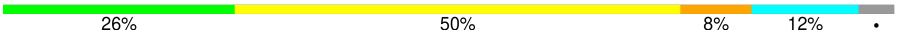


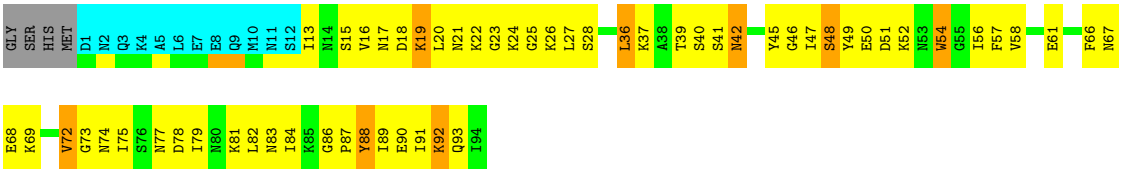


4.2.4 Score per residue for model 4

- Molecule 1: Hemolysin II

Chain D:

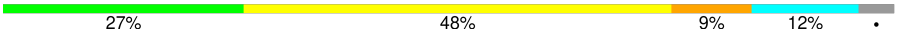


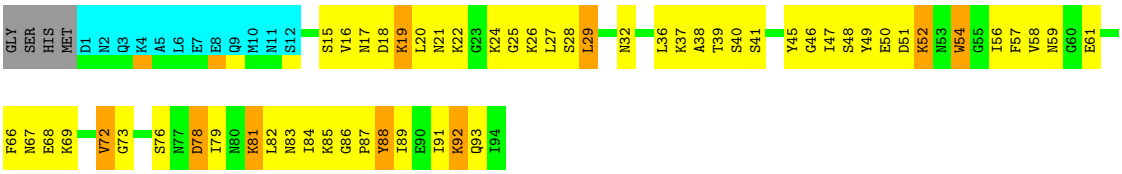


4.2.5 Score per residue for model 5

- Molecule 1: Hemolysin II

Chain D:





4.2.6 Score per residue for model 6

- Molecule 1: Hemolysin II

Chain D: 33% 42% 9% 12% •

GLY SER HIS MET D1 N2 Q3 K4 A5 L6 E7 E8 Q9 M10 N11 S12 I13 N14 S15 V16 K19 L20 N21 K22 G23 K24 G25 K26 L27 S28 L29 S30 M31 L36 K37 A38 T39 S40 S41 N42 Y45 G46 I47 S48 D51 K52 N53 W54 G55 I56 F57 V58 K62 V63

F66 N67 E68 V72 G73 S76 N77 D78 I79 N80 K81 L82 N83 I84 K85 G86 P87 Y88 I89 E90 I91 K92 Q93 I94

4.2.7 Score per residue for model 7

- Molecule 1: Hemolysin II

Chain D: 33% 44% 7% 12% •

GLY SER HIS MET D1 N2 Q3 K4 A5 L6 E7 E8 Q9 M10 N11 S12 V16 K19 L20 N21 K22 G23 K24 G25 K26 L27 S28 L29 L36 T39 S40 S41 N42 A43 G44 Y45 G46 I47 S48 Y49 E50 D51 K52 N53 W54 G55 I56 F57 V58 E61 F66 N67 E68 K69

S70 T71 V72 I75 D78 I79 N80 K81 L82 N83 I84 K85 G86 P87 Y88 I89 E90 I91 K92 Q93 I94

4.2.8 Score per residue for model 8

- Molecule 1: Hemolysin II

Chain D: 27% 51% 6% 12% •

GLY SER HIS MET D1 N2 Q3 K4 A5 L6 E7 E8 Q9 M10 N11 S12 I13 N14 S15 V16 N17 D18 K19 L20 N21 K22 G23 K24 G25 K26 L27 S28 N34 Q35 L36 T39 S40 S41 G44 Y45 G46 I47 S48 Y49 E50 D51 K52 N53 W54 G55 I56 F57 V58 N59 G60 E61 K62

F66 N67 E68 K69 V72 G73 N74 I75 S76 N77 D78 I79 N80 K81 L82 N83 I84 K85 G86 P87 Y88 I89 E90 I91 K92 Q93 I94

4.2.9 Score per residue for model 9

- Molecule 1: Hemolysin II

Chain D: 32% 44% 7% • 12% •

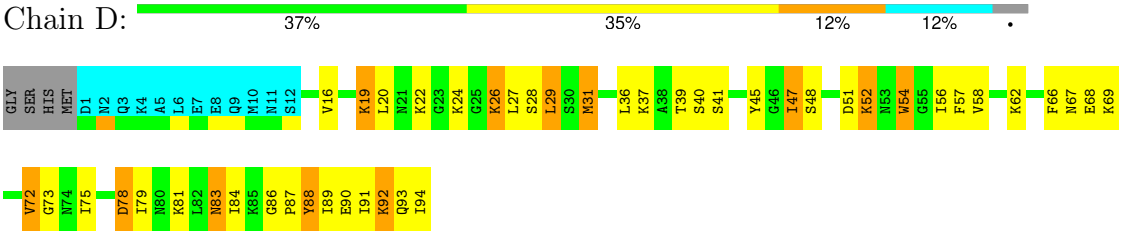
GLY SER HIS MET D1 N2 Q3 K4 A5 L6 E7 E8 Q9 M10 N11 S12 S15 V16 N17 D18 K19 L20 N21 K22 G23 K24 G25 K26 L27 S28 N32 L36 T39 S40 S41 N42 Y45 G46 I47 S48 Y49 E50 D51 K52 N53 W54 G55 I56 F57 V58 F66 N67 E68 K69

V72 G73 S76 N77 D78 I79 N80 K81 L82 N83 I84 K85 G86 P87 Y88 I89 E90 I91 K92 Q93 I94

4.2.10 Score per residue for model 10

- Molecule 1: Hemolysin II

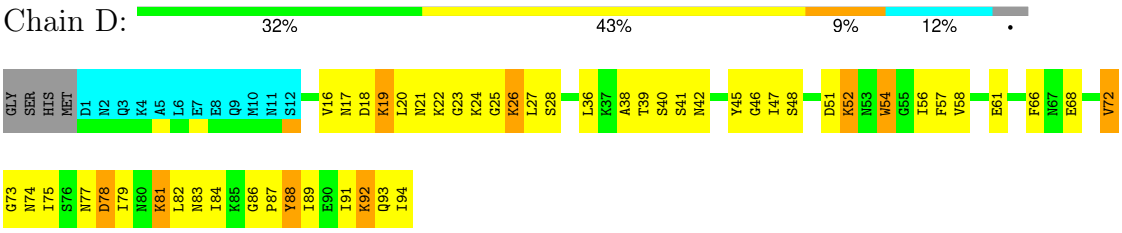
Chain D:



4.2.11 Score per residue for model 11

- Molecule 1: Hemolysin II

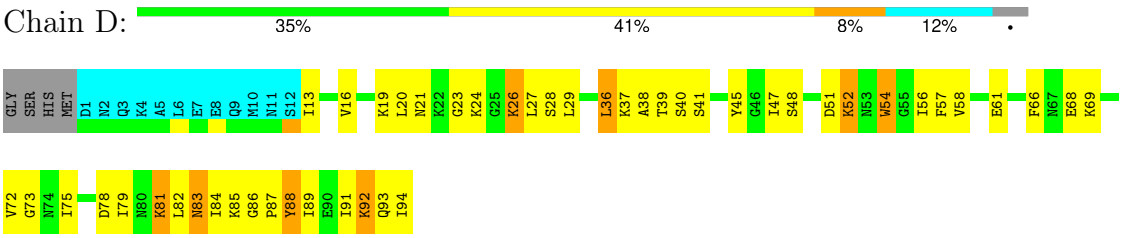
Chain D:



4.2.12 Score per residue for model 12

- Molecule 1: Hemolysin II

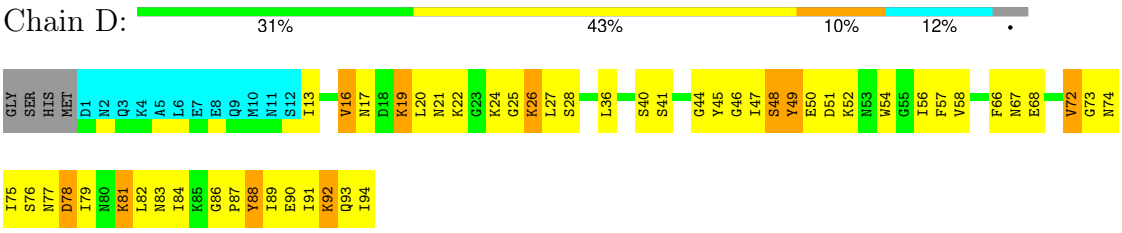
Chain D:



4.2.13 Score per residue for model 13

- Molecule 1: Hemolysin II

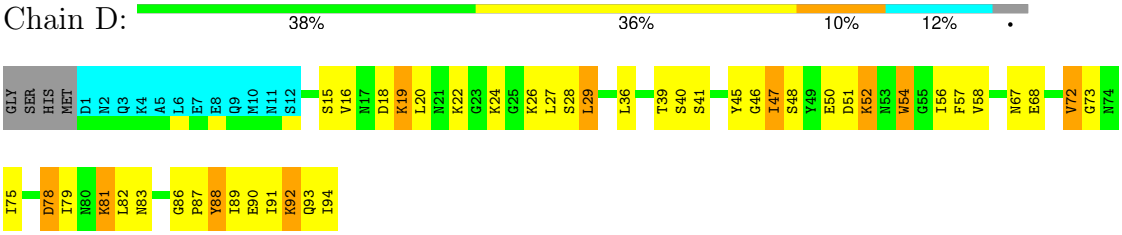
Chain D:



4.2.14 Score per residue for model 14

- Molecule 1: Hemolysin II

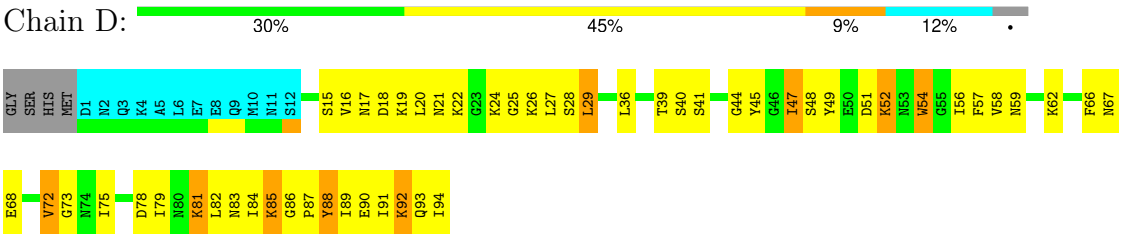
Chain D:



4.2.15 Score per residue for model 15

- Molecule 1: Hemolysin II

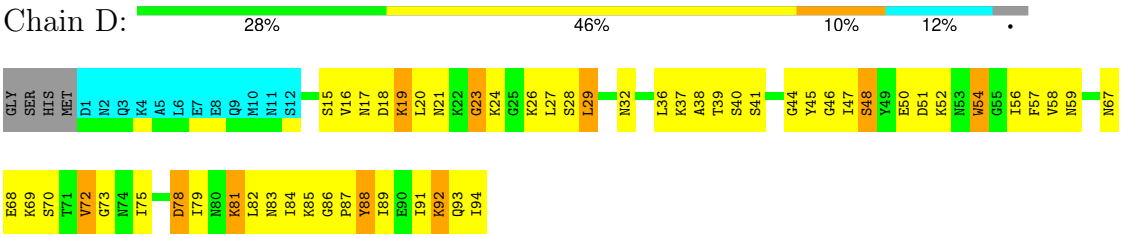
Chain D:



4.2.16 Score per residue for model 16

- Molecule 1: Hemolysin II

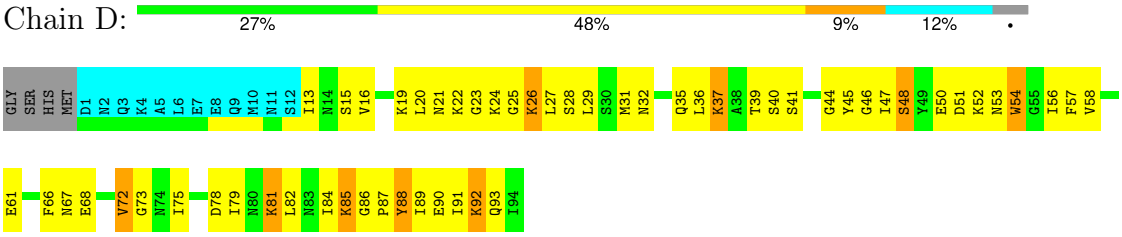
Chain D:



4.2.17 Score per residue for model 17

- Molecule 1: Hemolysin II

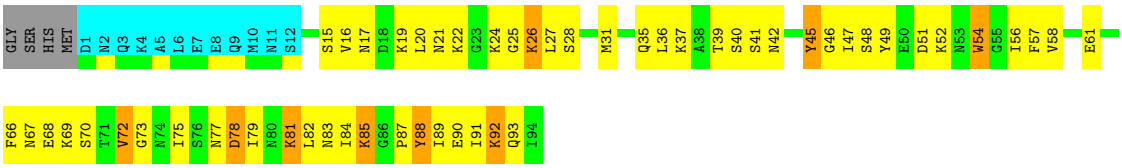
Chain D:



4.2.18 Score per residue for model 18

- Molecule 1: Hemolysin II

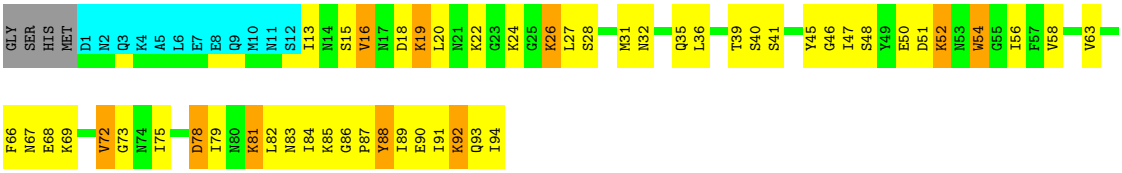
Chain D: 28% 47% 9% 12% •



4.2.19 Score per residue for model 19

- Molecule 1: Hemolysin II

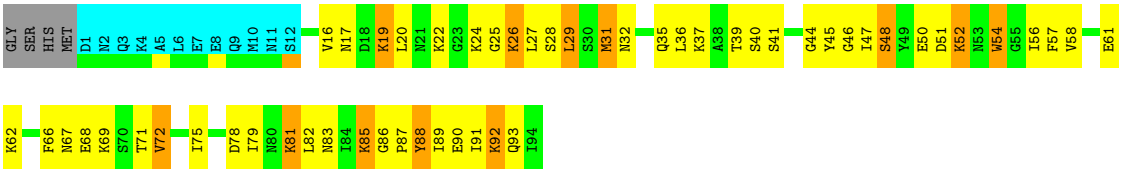
Chain D: 31% 43% 10% 12% •



4.2.20 Score per residue for model 20

- Molecule 1: Hemolysin II

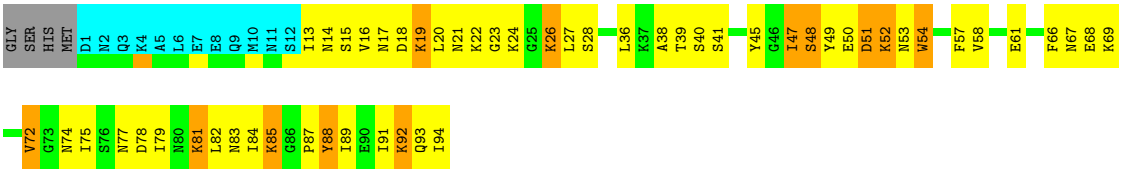
Chain D: 29% 43% 12% 12% •



4.2.21 Score per residue for model 21

- Molecule 1: Hemolysin II

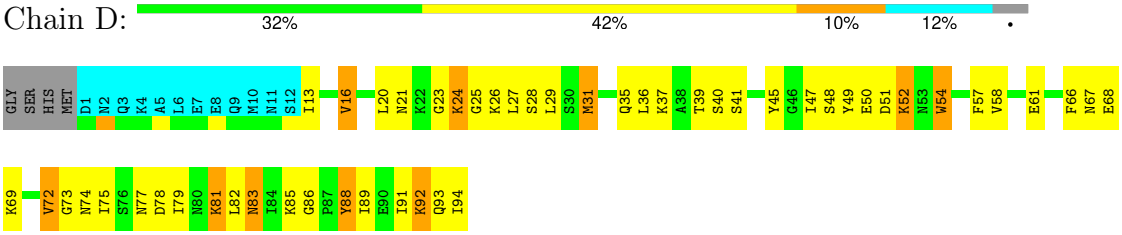
Chain D: 29% 43% 12% 12% •



4.2.22 Score per residue for model 22

- Molecule 1: Hemolysin II

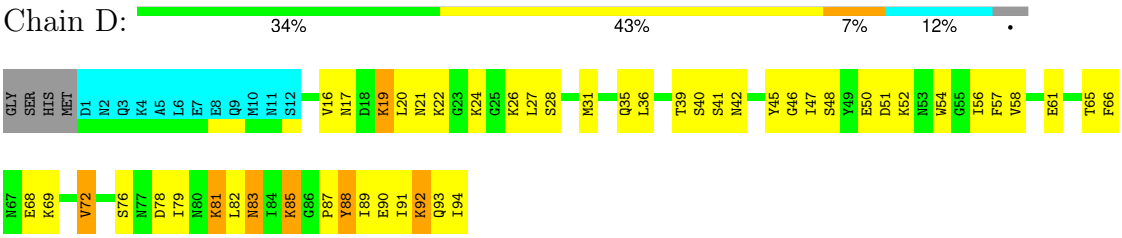
Chain D:



4.2.23 Score per residue for model 23

- Molecule 1: Hemolysin II

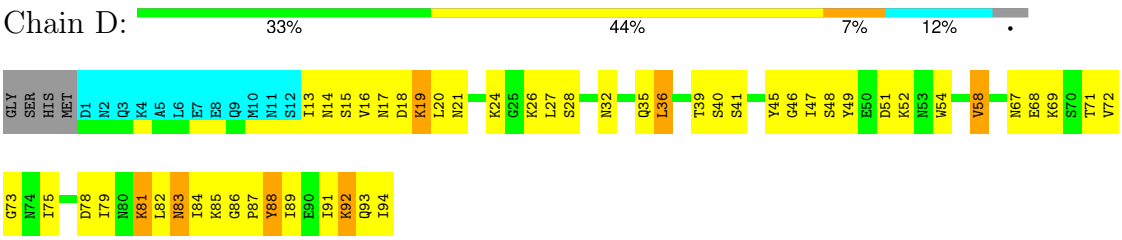
Chain D:



4.2.24 Score per residue for model 24

- Molecule 1: Hemolysin II

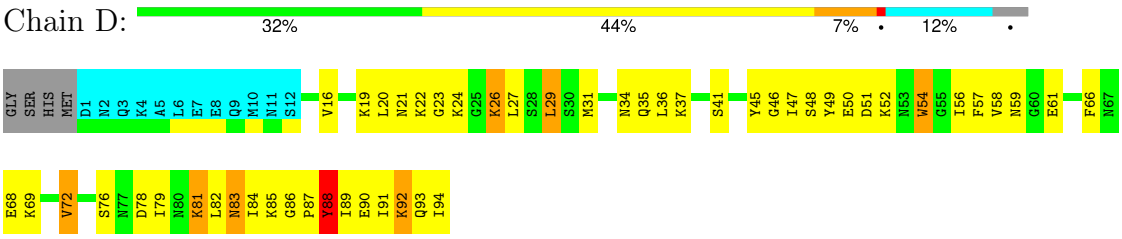
Chain D:



4.2.25 Score per residue for model 25

- Molecule 1: Hemolysin II

Chain D:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 25 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
XPLOR-NIH	structure calculation	
ARIA	refinement	2.3
TALOS-N	geometry optimization	

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	1123
Number of shifts mapped to atoms	1123
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality (i)

6.1 Standard geometry (i)

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	D	636	641	641	59±4
All	All	15900	16025	16025	1471

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 46.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:56:ILE:HG12	1:D:91:ILE:HG23	1.01	1.31	12	13
1:D:78:ASP:HA	1:D:81:LYS:HD3	0.97	1.36	14	19
1:D:54:TRP:HZ3	1:D:91:ILE:HG22	0.94	1.22	8	13
1:D:78:ASP:HA	1:D:81:LYS:HG2	0.91	1.40	10	3
1:D:52:LYS:HG2	1:D:68:GLU:HB2	0.90	1.42	11	1
1:D:20:LEU:HB3	1:D:27:LEU:HB3	0.89	1.42	4	24
1:D:25:GLY:HA2	1:D:42:ASN:HD21	0.89	1.27	2	3
1:D:47:ILE:HG13	1:D:68:GLU:HB2	0.87	1.44	23	5
1:D:47:ILE:HG13	1:D:68:GLU:HB3	0.87	1.45	15	4
1:D:36:LEU:HB2	1:D:85:LYS:HB2	0.87	1.46	7	5
1:D:54:TRP:CZ3	1:D:91:ILE:HG22	0.84	2.08	12	13
1:D:78:ASP:HA	1:D:81:LYS:HE3	0.83	1.50	1	1
1:D:57:PHE:HB2	1:D:90:GLU:HB3	0.80	1.51	7	6
1:D:47:ILE:HG12	1:D:68:GLU:HB3	0.80	1.54	25	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:47:ILE:HG13	1:D:68:GLU:CB	0.79	2.07	3	6
1:D:76:SER:HA	1:D:79:ILE:HG12	0.78	1.56	25	6
1:D:56:ILE:HG21	1:D:84:ILE:HG21	0.78	1.54	12	2
1:D:19:LYS:N	1:D:19:LYS:HE2	0.78	1.93	4	2
1:D:36:LEU:HD11	1:D:79:ILE:HG22	0.77	1.56	20	21
1:D:22:LYS:HD2	1:D:47:ILE:HD12	0.76	1.57	11	7
1:D:25:GLY:HA2	1:D:42:ASN:ND2	0.76	1.95	18	7
1:D:86:GLY:H	1:D:89:ILE:HD11	0.76	1.40	12	12
1:D:20:LEU:HD13	1:D:27:LEU:HD23	0.74	1.60	15	7
1:D:58:VAL:HA	1:D:88:TYR:O	0.72	1.85	13	25
1:D:24:LYS:HB3	1:D:46:GLY:O	0.72	1.85	23	19
1:D:31:MET:HA	1:D:35:GLN:O	0.71	1.85	18	5
1:D:47:ILE:HD11	1:D:68:GLU:HG3	0.71	1.63	24	1
1:D:24:LYS:HG2	1:D:45:TYR:HB3	0.71	1.62	3	8
1:D:58:VAL:HG22	1:D:89:ILE:HG12	0.71	1.59	21	11
1:D:50:GLU:HB3	1:D:52:LYS:HE3	0.71	1.62	20	3
1:D:26:LYS:HD2	1:D:41:SER:HB3	0.71	1.61	6	10
1:D:40:SER:OG	1:D:73:GLY:HA2	0.71	1.86	22	14
1:D:22:LYS:HE2	1:D:22:LYS:HA	0.70	1.64	6	1
1:D:24:LYS:HE2	1:D:48:SER:HA	0.69	1.64	4	3
1:D:47:ILE:CG1	1:D:68:GLU:HB3	0.69	2.17	6	15
1:D:47:ILE:H	1:D:47:ILE:HD12	0.69	1.47	10	9
1:D:78:ASP:HA	1:D:81:LYS:CD	0.68	2.17	13	19
1:D:84:ILE:HG21	1:D:91:ILE:HD11	0.68	1.63	19	2
1:D:24:LYS:HE3	1:D:48:SER:HA	0.68	1.65	16	1
1:D:52:LYS:HG3	1:D:68:GLU:HB2	0.66	1.64	19	1
1:D:89:ILE:HG22	1:D:91:ILE:HG13	0.66	1.65	15	11
1:D:26:LYS:HD2	1:D:41:SER:HB2	0.66	1.65	10	6
1:D:21:ASN:OD1	1:D:26:LYS:HB2	0.66	1.90	17	12
1:D:36:LEU:HB2	1:D:85:LYS:HG2	0.66	1.66	16	2
1:D:78:ASP:HA	1:D:81:LYS:CG	0.66	2.19	10	3
1:D:78:ASP:CA	1:D:81:LYS:HG2	0.66	2.21	4	3
1:D:92:LYS:HE3	1:D:94:ILE:HG22	0.66	1.66	22	3
1:D:20:LEU:HD12	1:D:29:LEU:HD11	0.66	1.68	15	2
1:D:28:SER:HB2	1:D:39:THR:OG1	0.65	1.92	1	11
1:D:47:ILE:CG1	1:D:68:GLU:HB2	0.65	2.21	23	5
1:D:16:VAL:HA	1:D:19:LYS:HE2	0.65	1.67	13	11
1:D:58:VAL:HB	1:D:87:PRO:O	0.65	1.91	12	1
1:D:56:ILE:HD13	1:D:84:ILE:HG12	0.65	1.68	17	4
1:D:36:LEU:HD12	1:D:83:ASN:HA	0.64	1.69	11	4
1:D:52:LYS:O	1:D:67:ASN:HA	0.64	1.93	9	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:20:LEU:O	1:D:26:LYS:HA	0.64	1.93	16	20
1:D:24:LYS:HG3	1:D:45:TYR:HB3	0.63	1.70	21	15
1:D:74:ASN:HA	1:D:77:ASN:HD22	0.63	1.51	13	6
1:D:58:VAL:HG12	1:D:89:ILE:HG12	0.63	1.68	12	1
1:D:57:PHE:CE2	1:D:92:LYS:HE2	0.63	2.28	18	2
1:D:57:PHE:HB2	1:D:90:GLU:HB2	0.63	1.69	4	4
1:D:57:PHE:CE1	1:D:92:LYS:HE2	0.63	2.27	16	3
1:D:67:ASN:OD1	1:D:69:LYS:HG3	0.62	1.94	3	1
1:D:67:ASN:HD22	1:D:69:LYS:HB2	0.62	1.53	9	5
1:D:52:LYS:CE	1:D:68:GLU:HB2	0.62	2.24	18	1
1:D:26:LYS:CD	1:D:41:SER:HB2	0.62	2.25	3	8
1:D:22:LYS:HD3	1:D:47:ILE:HG23	0.62	1.70	18	2
1:D:15:SER:HA	1:D:18:ASP:OD2	0.62	1.94	5	4
1:D:20:LEU:HD13	1:D:27:LEU:HG	0.62	1.70	25	17
1:D:16:VAL:HG11	1:D:29:LEU:HD11	0.62	1.70	16	1
1:D:52:LYS:HD3	1:D:68:GLU:HB2	0.62	1.70	1	6
1:D:15:SER:O	1:D:19:LYS:HE3	0.62	1.94	3	2
1:D:26:LYS:CG	1:D:41:SER:HB3	0.62	2.25	24	14
1:D:54:TRP:HB2	1:D:66:PHE:O	0.61	1.95	23	18
1:D:50:GLU:HB2	1:D:52:LYS:HE2	0.61	1.70	8	1
1:D:51:ASP:C	1:D:52:LYS:HD2	0.61	2.16	10	21
1:D:27:LEU:HD13	1:D:76:SER:HB2	0.61	1.72	6	3
1:D:51:ASP:HA	1:D:69:LYS:HD3	0.61	1.72	24	1
1:D:76:SER:HA	1:D:79:ILE:CG1	0.61	2.25	25	5
1:D:37:LYS:HA	1:D:37:LYS:HE2	0.61	1.72	5	1
1:D:58:VAL:HG13	1:D:87:PRO:O	0.61	1.96	15	22
1:D:26:LYS:CD	1:D:41:SER:HB3	0.61	2.25	4	17
1:D:26:LYS:HG3	1:D:41:SER:HB3	0.61	1.72	17	16
1:D:47:ILE:HG12	1:D:52:LYS:HD3	0.61	1.73	12	5
1:D:44:GLY:O	1:D:71:THR:HB	0.61	1.96	3	3
1:D:50:GLU:O	1:D:69:LYS:HG2	0.61	1.95	5	8
1:D:16:VAL:HA	1:D:19:LYS:CE	0.61	2.26	23	10
1:D:92:LYS:HD3	1:D:93:GLN:O	0.60	1.96	19	5
1:D:52:LYS:HE2	1:D:68:GLU:CB	0.60	2.26	16	1
1:D:44:GLY:HA2	1:D:73:GLY:HA3	0.60	1.70	13	6
1:D:51:ASP:HA	1:D:69:LYS:CG	0.60	2.27	7	6
1:D:84:ILE:HG22	1:D:89:ILE:HD13	0.60	1.74	1	7
1:D:92:LYS:HE2	1:D:94:ILE:HG22	0.60	1.73	23	12
1:D:67:ASN:ND2	1:D:69:LYS:HB2	0.60	2.11	20	5
1:D:57:PHE:CE1	1:D:62:LYS:HG2	0.60	2.32	10	1
1:D:27:LEU:HB2	1:D:72:VAL:CG1	0.59	2.27	8	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:19:LYS:HB3	1:D:54:TRP:CZ2	0.59	2.32	12	1
1:D:54:TRP:NE1	1:D:93:GLN:HB3	0.59	2.13	11	19
1:D:25:GLY:CA	1:D:42:ASN:HD21	0.59	2.09	2	3
1:D:51:ASP:C	1:D:52:LYS:HD3	0.59	2.18	18	3
1:D:26:LYS:HG3	1:D:41:SER:HB2	0.59	1.75	20	5
1:D:16:VAL:HG13	1:D:17:ASN:ND2	0.59	2.13	8	5
1:D:20:LEU:HD22	1:D:27:LEU:HD23	0.59	1.74	11	3
1:D:81:LYS:HB3	1:D:81:LYS:NZ	0.59	2.13	14	1
1:D:78:ASP:O	1:D:82:LEU:HD23	0.58	1.98	16	24
1:D:86:GLY:HA2	1:D:89:ILE:HD11	0.58	1.75	5	6
1:D:52:LYS:HG2	1:D:68:GLU:OE1	0.58	1.99	25	3
1:D:27:LEU:HB2	1:D:72:VAL:HG11	0.58	1.74	4	8
1:D:21:ASN:HA	1:D:26:LYS:CB	0.58	2.29	9	17
1:D:16:VAL:O	1:D:20:LEU:HG	0.58	1.98	16	16
1:D:52:LYS:CG	1:D:68:GLU:HB2	0.58	2.28	19	1
1:D:34:ASN:O	1:D:85:LYS:HE3	0.57	1.98	8	3
1:D:72:VAL:HA	1:D:75:ILE:HD12	0.57	1.75	21	5
1:D:51:ASP:CB	1:D:69:LYS:HD3	0.57	2.28	24	1
1:D:92:LYS:HE3	1:D:93:GLN:O	0.57	1.99	5	2
1:D:41:SER:O	1:D:42:ASN:HB3	0.57	1.99	23	1
1:D:20:LEU:HD13	1:D:27:LEU:CG	0.57	2.29	25	19
1:D:56:ILE:HG23	1:D:91:ILE:HG12	0.57	1.75	3	11
1:D:75:ILE:O	1:D:79:ILE:HG13	0.57	2.00	21	18
1:D:51:ASP:HB2	1:D:69:LYS:HD2	0.57	1.73	23	4
1:D:67:ASN:O	1:D:75:ILE:HD11	0.57	2.00	22	6
1:D:19:LYS:O	1:D:22:LYS:HE3	0.57	1.99	14	5
1:D:17:ASN:OD1	1:D:28:SER:HA	0.56	1.99	16	4
1:D:78:ASP:HA	1:D:81:LYS:CE	0.56	2.29	1	1
1:D:27:LEU:HD13	1:D:28:SER:N	0.56	2.15	17	1
1:D:20:LEU:O	1:D:22:LYS:HG3	0.56	2.01	3	1
1:D:50:GLU:CB	1:D:52:LYS:HE3	0.56	2.30	20	3
1:D:56:ILE:HA	1:D:90:GLU:O	0.56	2.00	19	2
1:D:52:LYS:HE3	1:D:68:GLU:HB2	0.56	1.78	18	1
1:D:92:LYS:HE3	1:D:94:ILE:CG2	0.56	2.31	15	2
1:D:92:LYS:HG2	1:D:93:GLN:O	0.56	2.00	4	18
1:D:78:ASP:CA	1:D:81:LYS:HE3	0.55	2.28	1	1
1:D:50:GLU:HB3	1:D:52:LYS:HE2	0.55	1.77	17	4
1:D:54:TRP:CH2	1:D:92:LYS:HA	0.55	2.36	14	15
1:D:19:LYS:O	1:D:22:LYS:HE2	0.55	2.00	13	4
1:D:29:LEU:HA	1:D:37:LYS:O	0.55	2.01	12	11
1:D:13:ILE:O	1:D:16:VAL:HG12	0.55	2.02	13	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:51:ASP:HB2	1:D:69:LYS:HD3	0.55	1.79	24	1
1:D:51:ASP:O	1:D:52:LYS:HD2	0.54	2.02	23	5
1:D:17:ASN:ND2	1:D:28:SER:HA	0.54	2.17	5	1
1:D:51:ASP:O	1:D:52:LYS:HD3	0.54	2.02	7	1
1:D:32:ASN:O	1:D:35:GLN:HB2	0.54	2.03	19	1
1:D:19:LYS:N	1:D:19:LYS:HD2	0.54	2.17	8	6
1:D:57:PHE:HA	1:D:61:GLU:O	0.54	2.02	11	16
1:D:32:ASN:HB3	1:D:35:GLN:HB3	0.54	1.80	1	2
1:D:85:LYS:HE3	1:D:85:LYS:HA	0.54	1.80	17	1
1:D:89:ILE:CG2	1:D:91:ILE:HG13	0.54	2.33	22	7
1:D:22:LYS:HB3	1:D:22:LYS:NZ	0.54	2.18	21	2
1:D:25:GLY:HA3	1:D:45:TYR:O	0.53	2.03	17	11
1:D:92:LYS:HE2	1:D:94:ILE:CG2	0.53	2.33	23	10
1:D:50:GLU:HB2	1:D:52:LYS:HE3	0.53	1.80	1	1
1:D:47:ILE:HG13	1:D:52:LYS:HZ1	0.53	1.63	16	1
1:D:40:SER:HB2	1:D:73:GLY:HA2	0.53	1.79	16	1
1:D:42:ASN:ND2	1:D:45:TYR:HB2	0.53	2.19	4	4
1:D:59:ASN:HD21	1:D:87:PRO:HG2	0.53	1.62	25	2
1:D:47:ILE:HG12	1:D:68:GLU:CB	0.53	2.33	24	3
1:D:51:ASP:CA	1:D:69:LYS:HD3	0.53	2.34	24	1
1:D:52:LYS:HB2	1:D:68:GLU:CG	0.53	2.34	2	8
1:D:78:ASP:O	1:D:81:LYS:HG2	0.52	2.05	6	13
1:D:28:SER:HB3	1:D:39:THR:OG1	0.52	2.05	19	12
1:D:57:PHE:HD1	1:D:90:GLU:O	0.52	1.87	23	5
1:D:26:LYS:CG	1:D:41:SER:HB2	0.52	2.34	20	7
1:D:58:VAL:HG21	1:D:87:PRO:HD2	0.52	1.81	24	1
1:D:26:LYS:O	1:D:40:SER:HA	0.52	2.05	23	12
1:D:21:ASN:HA	1:D:26:LYS:HB2	0.52	1.82	22	3
1:D:22:LYS:HB2	1:D:22:LYS:NZ	0.52	2.19	10	1
1:D:77:ASN:O	1:D:81:LYS:HD3	0.52	2.05	18	2
1:D:22:LYS:CE	1:D:47:ILE:HA	0.52	2.35	15	1
1:D:51:ASP:CB	1:D:69:LYS:HD2	0.52	2.34	19	4
1:D:15:SER:HA	1:D:18:ASP:OD1	0.51	2.05	4	3
1:D:17:ASN:HB3	1:D:21:ASN:ND2	0.51	2.20	21	2
1:D:50:GLU:CB	1:D:52:LYS:HE2	0.51	2.35	17	3
1:D:22:LYS:NZ	1:D:47:ILE:HA	0.51	2.19	10	1
1:D:57:PHE:HD2	1:D:90:GLU:O	0.51	1.88	1	6
1:D:54:TRP:HZ3	1:D:91:ILE:HG23	0.51	1.66	22	7
1:D:50:GLU:HB2	1:D:52:LYS:NZ	0.51	2.19	16	1
1:D:20:LEU:HD13	1:D:27:LEU:CD2	0.51	2.33	15	6
1:D:56:ILE:HD13	1:D:84:ILE:HD13	0.51	1.81	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:51:ASP:HA	1:D:69:LYS:CD	0.51	2.35	24	1
1:D:36:LEU:HB2	1:D:84:ILE:O	0.51	2.06	13	1
1:D:37:LYS:NZ	1:D:37:LYS:HB3	0.51	2.21	17	4
1:D:40:SER:HB3	1:D:73:GLY:HA2	0.51	1.82	4	3
1:D:16:VAL:HA	1:D:19:LYS:HE3	0.51	1.82	7	1
1:D:53:ASN:HA	1:D:67:ASN:OD1	0.51	2.05	21	2
1:D:36:LEU:C	1:D:36:LEU:HD13	0.51	2.27	20	21
1:D:85:LYS:C	1:D:89:ILE:HD11	0.50	2.26	18	2
1:D:24:LYS:HE3	1:D:45:TYR:HD1	0.50	1.66	2	2
1:D:36:LEU:HG	1:D:84:ILE:O	0.50	2.07	11	4
1:D:69:LYS:HB3	1:D:69:LYS:NZ	0.50	2.22	8	4
1:D:22:LYS:HE3	1:D:47:ILE:HA	0.50	1.83	15	1
1:D:56:ILE:CG1	1:D:91:ILE:HG23	0.50	2.22	12	6
1:D:84:ILE:HD12	1:D:84:ILE:H	0.50	1.67	10	1
1:D:20:LEU:CB	1:D:27:LEU:HB3	0.49	2.37	17	1
1:D:59:ASN:OD1	1:D:87:PRO:HG2	0.49	2.08	16	2
1:D:90:GLU:HG2	1:D:92:LYS:HD2	0.49	1.85	18	1
1:D:89:ILE:HD12	1:D:89:ILE:N	0.49	2.22	4	7
1:D:36:LEU:HB3	1:D:83:ASN:HD22	0.49	1.68	24	3
1:D:16:VAL:CG2	1:D:91:ILE:HB	0.49	2.37	12	1
1:D:26:LYS:NZ	1:D:26:LYS:HB3	0.49	2.23	21	10
1:D:27:LEU:HD11	1:D:38:ALA:HB1	0.49	1.83	21	1
1:D:22:LYS:HA	1:D:22:LYS:CE	0.48	2.38	6	1
1:D:40:SER:CB	1:D:73:GLY:HA2	0.48	2.38	6	1
1:D:19:LYS:HB3	1:D:54:TRP:HZ2	0.48	1.65	12	1
1:D:57:PHE:CE1	1:D:92:LYS:NZ	0.48	2.77	9	2
1:D:20:LEU:CD1	1:D:29:LEU:HD11	0.48	2.38	6	6
1:D:36:LEU:HG	1:D:84:ILE:N	0.48	2.23	5	4
1:D:22:LYS:CD	1:D:47:ILE:HD12	0.48	2.39	5	1
1:D:84:ILE:HD12	1:D:84:ILE:N	0.48	2.24	10	6
1:D:17:ASN:O	1:D:21:ASN:HB2	0.48	2.09	15	1
1:D:35:GLN:HB3	1:D:37:LYS:HE2	0.48	1.86	18	1
1:D:52:LYS:HB2	1:D:68:GLU:HB2	0.47	1.84	18	2
1:D:35:GLN:O	1:D:85:LYS:HD3	0.47	2.09	19	1
1:D:85:LYS:C	1:D:85:LYS:HE3	0.47	2.29	18	2
1:D:52:LYS:HE2	1:D:68:GLU:HB2	0.47	1.85	16	1
1:D:22:LYS:NZ	1:D:47:ILE:HG23	0.47	2.25	9	1
1:D:92:LYS:O	1:D:92:LYS:HD2	0.47	2.10	19	2
1:D:85:LYS:HE3	1:D:85:LYS:O	0.47	2.09	18	1
1:D:54:TRP:CE3	1:D:66:PHE:CZ	0.47	3.03	11	9
1:D:19:LYS:O	1:D:22:LYS:HG3	0.47	2.09	2	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:25:GLY:HA2	1:D:42:ASN:HD22	0.47	1.70	7	3
1:D:15:SER:O	1:D:19:LYS:HE2	0.47	2.10	17	2
1:D:54:TRP:O	1:D:65:THR:HA	0.47	2.10	23	1
1:D:85:LYS:O	1:D:85:LYS:HE3	0.47	2.10	21	3
1:D:47:ILE:CG1	1:D:52:LYS:HE3	0.47	2.40	18	1
1:D:51:ASP:HB3	1:D:69:LYS:HD2	0.47	1.87	19	1
1:D:47:ILE:HD11	1:D:69:LYS:HA	0.46	1.88	10	2
1:D:51:ASP:OD2	1:D:69:LYS:HE3	0.46	2.10	22	1
1:D:31:MET:SD	1:D:85:LYS:HE2	0.46	2.51	6	1
1:D:27:LEU:HB2	1:D:72:VAL:HG12	0.46	1.87	8	1
1:D:83:ASN:O	1:D:85:LYS:HE2	0.46	2.09	9	2
1:D:26:LYS:HG2	1:D:42:ASN:ND2	0.46	2.26	11	3
1:D:47:ILE:O	1:D:48:SER:HB2	0.46	2.10	7	3
1:D:47:ILE:HG13	1:D:52:LYS:HE3	0.46	1.88	8	1
1:D:54:TRP:CD1	1:D:93:GLN:HB3	0.46	2.46	13	4
1:D:51:ASP:HA	1:D:69:LYS:HD2	0.46	1.88	19	1
1:D:58:VAL:CG1	1:D:87:PRO:HD2	0.45	2.42	10	3
1:D:86:GLY:H	1:D:89:ILE:CD1	0.45	2.24	22	9
1:D:58:VAL:CG1	1:D:89:ILE:HG12	0.45	2.39	12	1
1:D:27:LEU:HD12	1:D:28:SER:H	0.45	1.71	6	4
1:D:50:GLU:CB	1:D:52:LYS:HD3	0.45	2.42	19	1
1:D:36:LEU:CD1	1:D:79:ILE:HG22	0.45	2.35	20	5
1:D:19:LYS:N	1:D:19:LYS:HD3	0.45	2.26	11	2
1:D:86:GLY:N	1:D:89:ILE:HD11	0.45	2.25	17	4
1:D:42:ASN:HD21	1:D:45:TYR:HB2	0.45	1.72	9	1
1:D:24:LYS:HE3	1:D:45:TYR:CD1	0.45	2.46	8	1
1:D:19:LYS:HD2	1:D:19:LYS:H	0.44	1.72	19	5
1:D:20:LEU:HD12	1:D:27:LEU:HD12	0.44	1.88	17	1
1:D:32:ASN:HB3	1:D:35:GLN:HB2	0.44	1.87	20	1
1:D:81:LYS:HD2	1:D:81:LYS:H	0.44	1.72	24	2
1:D:20:LEU:HB3	1:D:27:LEU:CB	0.44	2.30	4	1
1:D:16:VAL:CG1	1:D:29:LEU:HD11	0.44	2.41	16	1
1:D:23:GLY:O	1:D:26:LYS:HE3	0.44	2.12	16	1
1:D:47:ILE:CG1	1:D:52:LYS:HZ1	0.44	2.25	16	1
1:D:85:LYS:HE3	1:D:85:LYS:CA	0.44	2.42	17	1
1:D:24:LYS:HE3	1:D:45:TYR:CD2	0.44	2.48	7	1
1:D:15:SER:O	1:D:19:LYS:HD2	0.44	2.13	9	1
1:D:15:SER:O	1:D:18:ASP:HB2	0.44	2.13	24	2
1:D:57:PHE:HE2	1:D:92:LYS:HE2	0.44	1.69	18	1
1:D:56:ILE:O	1:D:63:VAL:HG12	0.44	2.13	6	2
1:D:92:LYS:C	1:D:92:LYS:HD2	0.44	2.33	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:22:LYS:HD2	1:D:47:ILE:CD1	0.44	2.42	13	1
1:D:57:PHE:HZ	1:D:94:ILE:HG21	0.43	1.73	23	4
1:D:75:ILE:O	1:D:78:ASP:HB2	0.43	2.14	4	5
1:D:18:ASP:C	1:D:19:LYS:HE2	0.43	2.33	4	2
1:D:92:LYS:C	1:D:92:LYS:CD	0.43	2.87	11	1
1:D:44:GLY:CA	1:D:73:GLY:HA3	0.43	2.43	13	1
1:D:24:LYS:HB3	1:D:47:ILE:O	0.43	2.13	22	3
1:D:67:ASN:O	1:D:70:SER:HB2	0.43	2.13	16	1
1:D:21:ASN:HA	1:D:26:LYS:HB3	0.43	1.91	23	3
1:D:36:LEU:HB3	1:D:83:ASN:ND2	0.43	2.28	10	3
1:D:31:MET:HB2	1:D:35:GLN:O	0.43	2.13	19	1
1:D:84:ILE:HG23	1:D:89:ILE:HD13	0.43	1.90	21	1
1:D:45:TYR:N	1:D:45:TYR:CD1	0.43	2.86	14	1
1:D:62:LYS:HB3	1:D:62:LYS:NZ	0.43	2.29	8	2
1:D:92:LYS:HD2	1:D:92:LYS:O	0.43	2.13	11	2
1:D:85:LYS:HE3	1:D:85:LYS:C	0.43	2.34	15	1
1:D:24:LYS:CD	1:D:48:SER:HA	0.42	2.43	3	2
1:D:47:ILE:HD12	1:D:47:ILE:N	0.42	2.25	10	1
1:D:24:LYS:HD3	1:D:48:SER:HA	0.42	1.89	17	2
1:D:47:ILE:HG21	1:D:52:LYS:HE3	0.42	1.90	12	1
1:D:28:SER:N	1:D:39:THR:O	0.42	2.52	4	1
1:D:79:ILE:HG23	1:D:84:ILE:HD13	0.42	1.90	17	2
1:D:52:LYS:HB3	1:D:52:LYS:NZ	0.42	2.28	11	1
1:D:88:TYR:CD2	1:D:88:TYR:N	0.42	2.88	1	1
1:D:28:SER:O	1:D:38:ALA:HA	0.42	2.14	3	6
1:D:16:VAL:HG21	1:D:91:ILE:HB	0.42	1.90	1	1
1:D:88:TYR:HD1	1:D:88:TYR:H	0.42	1.57	12	1
1:D:50:GLU:OE1	1:D:50:GLU:HA	0.42	2.15	22	1
1:D:36:LEU:HD11	1:D:79:ILE:CG2	0.42	2.42	1	1
1:D:59:ASN:ND2	1:D:88:TYR:HB2	0.42	2.30	5	1
1:D:31:MET:SD	1:D:31:MET:N	0.42	2.93	20	3
1:D:47:ILE:HD11	1:D:68:GLU:OE2	0.42	2.15	22	1
1:D:57:PHE:CE2	1:D:92:LYS:NZ	0.41	2.79	13	1
1:D:57:PHE:CE1	1:D:62:LYS:HB2	0.41	2.50	1	3
1:D:15:SER:C	1:D:19:LYS:HE3	0.41	2.36	3	1
1:D:49:TYR:CD1	1:D:49:TYR:N	0.41	2.88	13	1
1:D:51:ASP:HB3	1:D:69:LYS:HD3	0.41	1.93	16	1
1:D:20:LEU:HB2	1:D:27:LEU:HB3	0.41	1.91	17	1
1:D:47:ILE:H	1:D:47:ILE:CD1	0.41	2.20	6	1
1:D:84:ILE:CG2	1:D:89:ILE:HD13	0.41	2.45	17	1
1:D:67:ASN:O	1:D:70:SER:HB3	0.41	2.15	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:75:ILE:O	1:D:79:ILE:HG12	0.41	2.15	1	2
1:D:26:LYS:HE3	1:D:42:ASN:ND2	0.41	2.30	6	1
1:D:14:ASN:O	1:D:17:ASN:HB2	0.41	2.15	24	1
1:D:22:LYS:NZ	1:D:68:GLU:HG3	0.41	2.31	14	1
1:D:36:LEU:HD13	1:D:36:LEU:C	0.41	2.35	25	2
1:D:59:ASN:ND2	1:D:87:PRO:HG2	0.41	2.29	25	1
1:D:52:LYS:O	1:D:67:ASN:HB2	0.41	2.16	10	1
1:D:57:PHE:CE2	1:D:62:LYS:HB2	0.41	2.51	20	1
1:D:54:TRP:CZ3	1:D:91:ILE:HG23	0.41	2.49	22	1
1:D:56:ILE:O	1:D:62:LYS:HA	0.40	2.15	20	1
1:D:36:LEU:HG	1:D:84:ILE:HB	0.40	1.93	19	1
1:D:51:ASP:HA	1:D:69:LYS:HG2	0.40	1.94	7	1
1:D:92:LYS:CD	1:D:92:LYS:C	0.40	2.89	15	1
1:D:50:GLU:HB2	1:D:52:LYS:HZ3	0.40	1.74	16	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	81/98 (83%)	70±2 (86±3%)	9±3 (11±3%)	3±1 (3±1%)	6 37
All	All	2025/2450 (83%)	1744 (86%)	214 (11%)	67 (3%)	6 37

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	D	48	SER	25
1	D	88	TYR	25
1	D	23	GLY	12
1	D	71	THR	2
1	D	14	ASN	1
1	D	86	GLY	1
1	D	83	ASN	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	71/85 (84%)	62±2 (87±2%)	9±2 (13±2%)	7 49
All	All	1775/2125 (84%)	1546 (87%)	229 (13%)	7 49

All 25 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	D	72	VAL	25
1	D	92	LYS	25
1	D	81	LYS	21
1	D	54	TRP	20
1	D	83	ASN	19
1	D	19	LYS	17
1	D	49	TYR	14
1	D	52	LYS	13
1	D	29	LEU	11
1	D	26	LYS	11
1	D	85	LYS	11
1	D	78	ASP	9
1	D	47	ILE	6
1	D	32	ASN	5
1	D	42	ASN	4
1	D	88	TYR	3
1	D	36	LEU	3
1	D	31	MET	3
1	D	16	VAL	3
1	D	18	ASP	1
1	D	37	LYS	1
1	D	45	TYR	1
1	D	51	ASP	1
1	D	24	LYS	1
1	D	58	VAL	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1123
Number of shifts mapped to atoms	1123
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	93	-0.66 ± 0.14	Should be applied
$^{13}C_{\beta}$	84	-0.36 ± 0.14	None needed (< 0.5 ppm)
$^{13}C'$	94	-0.12 ± 0.18	None needed (< 0.5 ppm)
^{15}N	93	-0.13 ± 0.54	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 995 atoms were assigned a chemical shift out of a possible 1091. 0 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	417/417 (100%)	172/172 (100%)	164/164 (100%)	81/81 (100%)
Sidechain	545/606 (90%)	365/389 (94%)	165/191 (86%)	15/26 (58%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	33/68 (49%)	32/32 (100%)	0/35 (0%)	1/1 (100%)
Overall	995/1091 (91%)	569/593 (96%)	329/390 (84%)	97/108 (90%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1123 atoms were assigned a chemical shift out of a possible 1246. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	474/477 (99%)	194/196 (99%)	187/188 (99%)	93/93 (100%)
Sidechain	616/701 (88%)	413/448 (92%)	184/222 (83%)	19/31 (61%)
Aromatic	33/68 (49%)	32/32 (100%)	0/35 (0%)	1/1 (100%)
Overall	1123/1246 (90%)	639/676 (95%)	371/445 (83%)	113/125 (90%)

7.1.4 Statistically unusual chemical shifts (i)

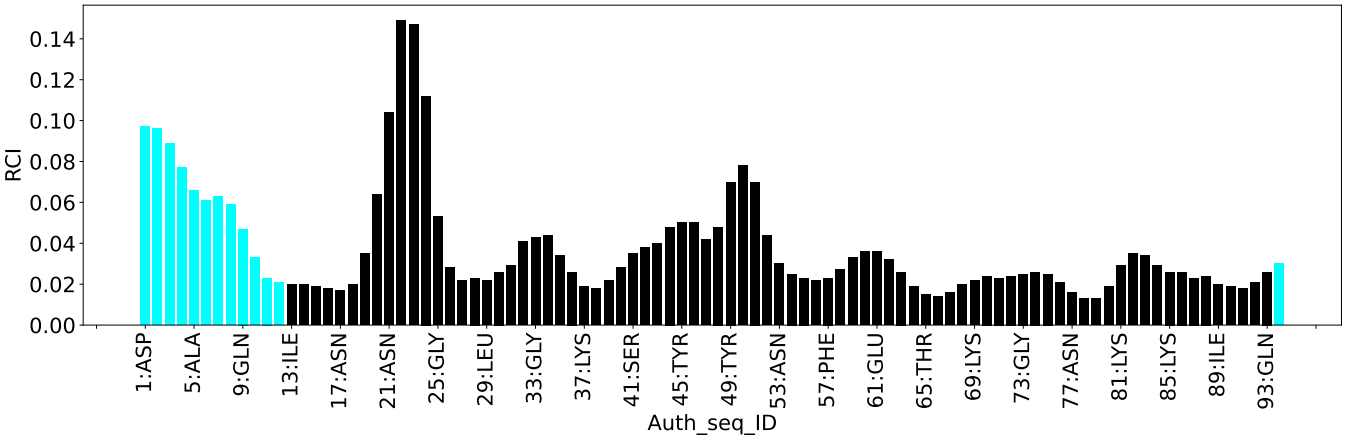
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	D	54	TRP	HB3	0.87	1.31 – 4.93	-6.2

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 D:


RCI
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
1:ASP
5:ALA
9:GLN
13:ILE
17:ASN
21:ASN
25:GLY
29:LEU
33:GLY
37:LYS
41:SER
45:TYR
49:TYR
53:ASN
57:PHE
61:GLU
65:THR
69:LYS
73:GLY
77:ASN
81:LYS
85:LYS
89:ILE
93:GLN
Auth_seq_ID