



Full wwPDB NMR Structure Validation Report ⓘ

Jul 19, 2023 – 06:04 AM EDT

PDB ID : 2L4Z
Title : NMR structure of fusion of CtIP (641-685) to LMO4-LIM1 (18-82)
Authors : Liew, C.; Stokes, P.H.; Kwan, A.H.; Matthews, J.M.
Deposited on : 2010-10-22

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 : 4.02b-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) : 2.34

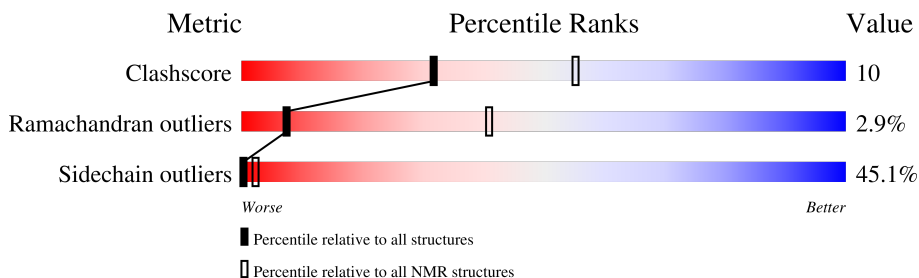
1 Overall quality at a glance

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	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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	123	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:663-A:675, A:20-A:82 (76)	0.96	19

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 3 single-model clusters were found.

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

3 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 1779 atoms, of which 866 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA endonuclease RBBP8,LIM domain transcription factor LMO4.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	121	1777	560	866	161	180	10	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	639	GLY	-	expression tag	UNP Q99708
A	640	SER	-	expression tag	UNP Q99708
A	901	GLY	-	linker	UNP Q99708
A	902	GLY	-	linker	UNP Q99708
A	903	SER	-	linker	UNP Q99708
A	904	GLY	-	linker	UNP Q99708
A	905	GLY	-	linker	UNP Q99708
A	906	HIS	-	linker	UNP Q99708
A	907	MET	-	linker	UNP Q99708
A	908	GLY	-	linker	UNP Q99708
A	909	SER	-	linker	UNP Q99708
A	910	GLY	-	linker	UNP Q99708
A	911	GLY	-	linker	UNP Q99708
A	52	SER	CYS	engineered mutation	UNP P61969
A	64	SER	CYS	engineered mutation	UNP P61969

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

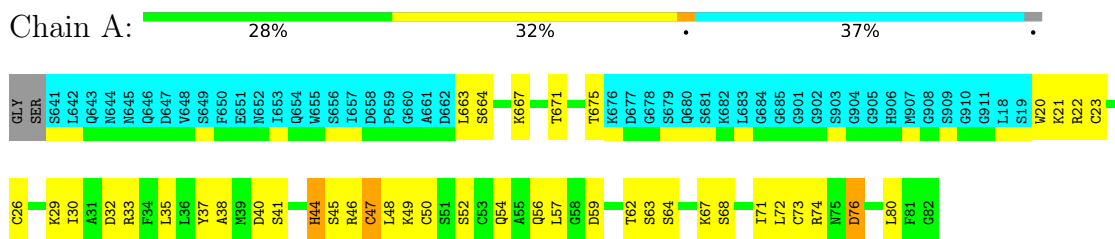
Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: DNA endonuclease RBBP8,LIM domain transcription factor LMO4

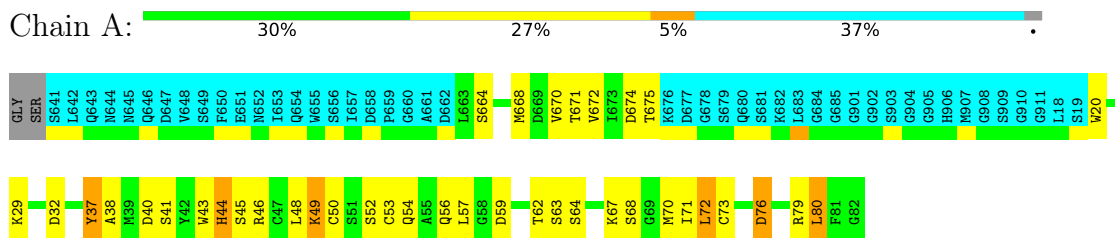


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

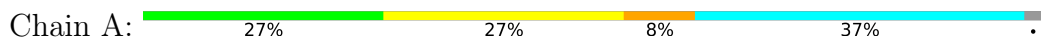
4.2.1 Score per residue for model 1

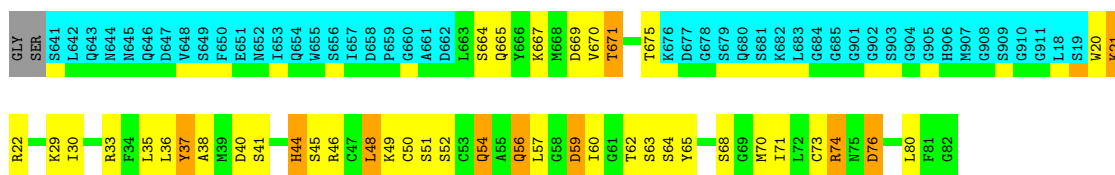
- Molecule 1: DNA endonuclease RBBP8,LIM domain transcription factor LMO4



4.2.2 Score per residue for model 2

- Molecule 1: DNA endonuclease RBBP8,LIM domain transcription factor LMO4

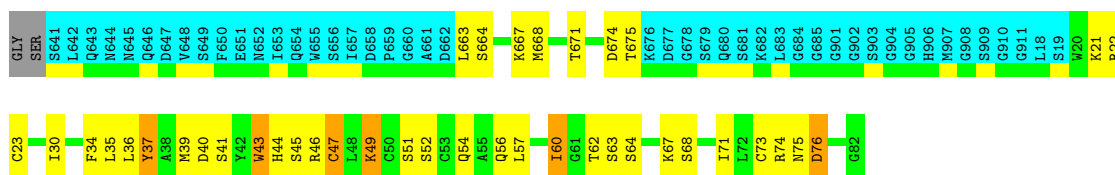




4.2.3 Score per residue for model 3

- Molecule 1: DNA endonuclease RBBP8,LIM domain transcription factor LMO4

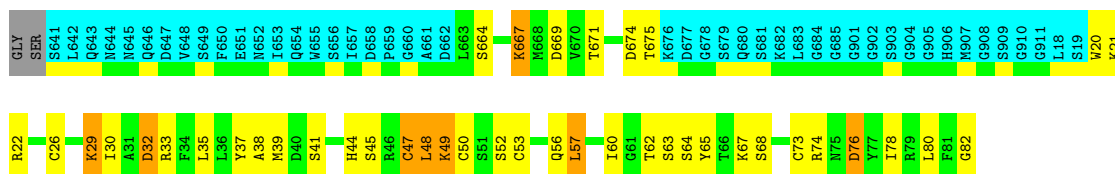
Chain A: 29% 28% 5% 37%



4.2.4 Score per residue for model 4

- Molecule 1: DNA endonuclease RBBP8,LIM domain transcription factor LMO4

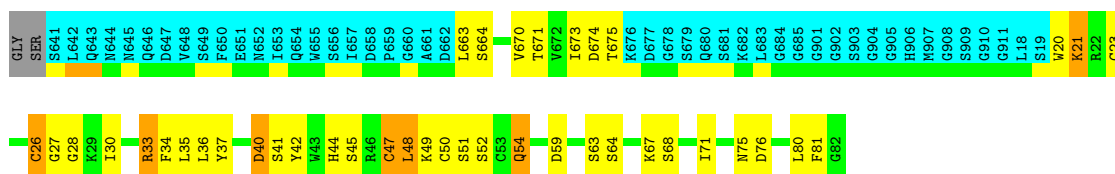
Chain A: 28% 28% 7% 37%



4.2.5 Score per residue for model 5

- Molecule 1: DNA endonuclease RBBP8,LIM domain transcription factor LMO4

Chain A: 28% 28% 6% 37%

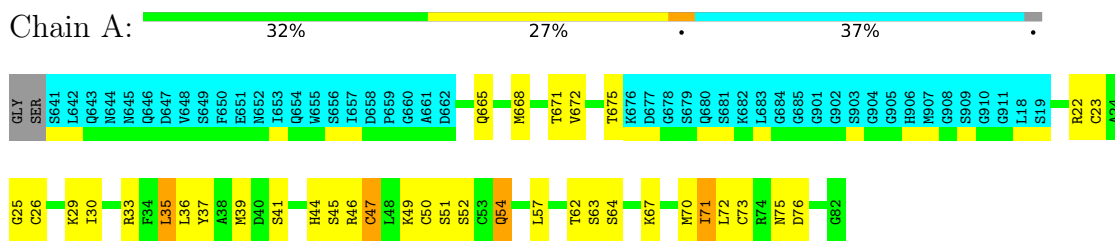


4.2.6 Score per residue for model 6

- Molecule 1: DNA endonuclease RBBP8,LIM domain transcription factor LMO4

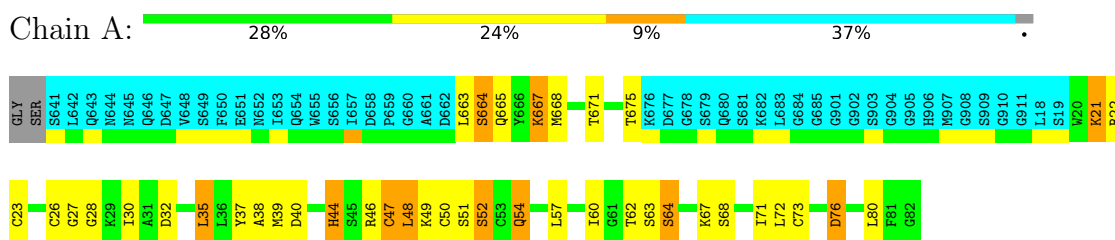
4.2.10 Score per residue for model 10

- Molecule 1: DNA endonuclease RBBP8,LIM domain transcription factor LMO4



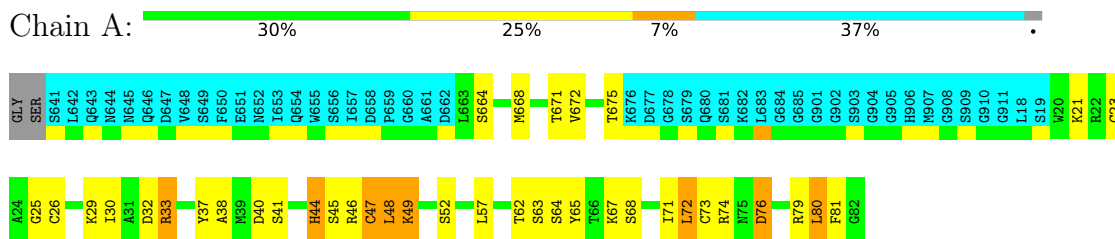
4.2.11 Score per residue for model 11

- Molecule 1: DNA endonuclease RBBP8,LIM domain transcription factor LMO4



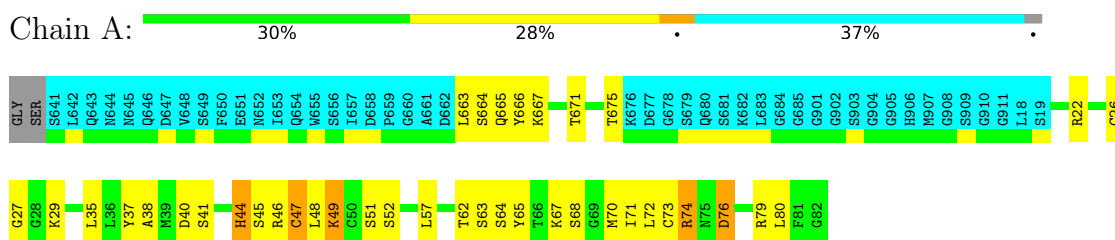
4.2.12 Score per residue for model 12

- Molecule 1: DNA endonuclease RBBP8,LIM domain transcription factor LMO4



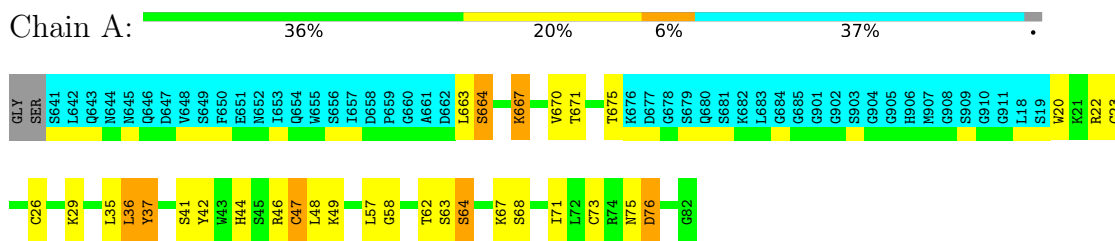
4.2.13 Score per residue for model 13

- Molecule 1: DNA endonuclease RBBP8,LIM domain transcription factor LMO4



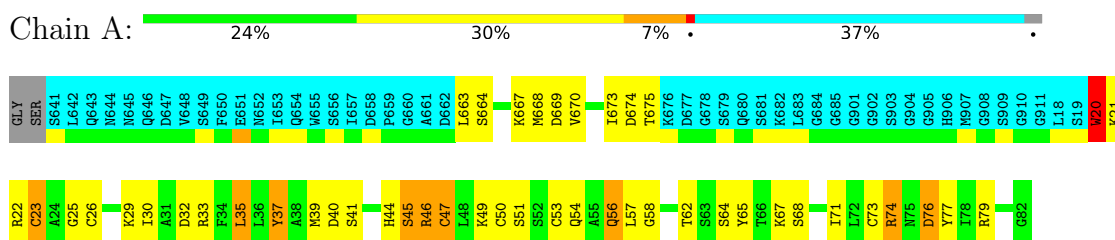
4.2.14 Score per residue for model 14

- Molecule 1: DNA endonuclease RBBP8,LIM domain transcription factor LMO4



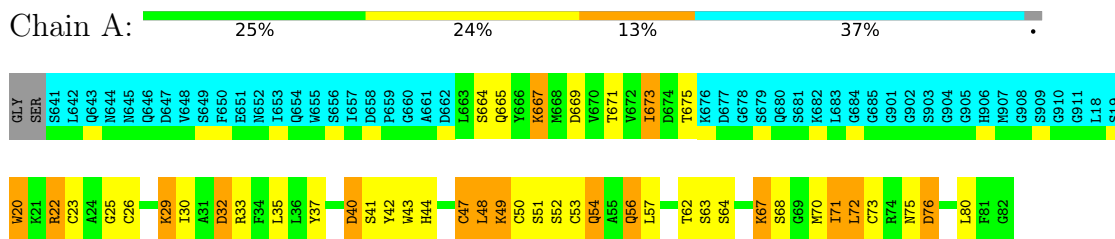
4.2.15 Score per residue for model 15

- Molecule 1: DNA endonuclease RBBP8,LIM domain transcription factor LMO4



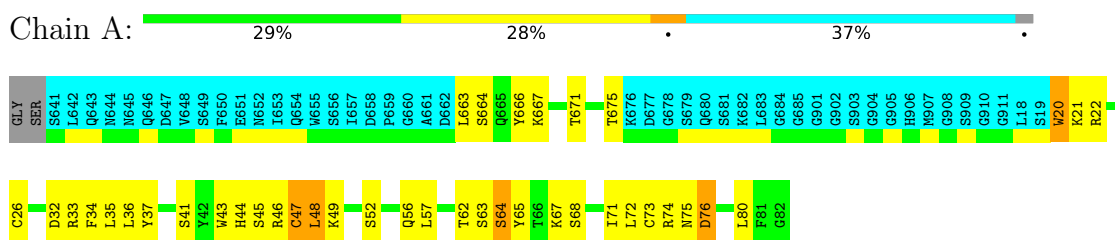
4.2.16 Score per residue for model 16

- Molecule 1: DNA endonuclease RBBP8,LIM domain transcription factor LMO4



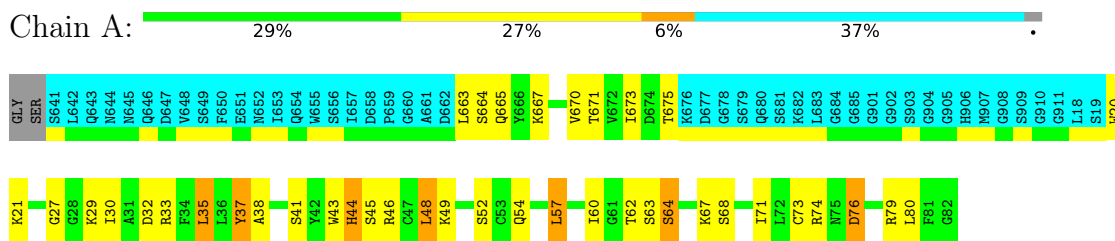
4.2.17 Score per residue for model 17

- Molecule 1: DNA endonuclease RBBP8,LIM domain transcription factor LMO4



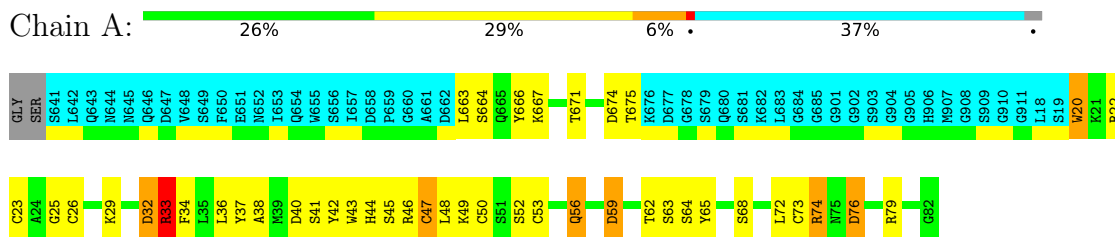
4.2.18 Score per residue for model 18

- Molecule 1: DNA endonuclease RBBP8,LIM domain transcription factor LMO4



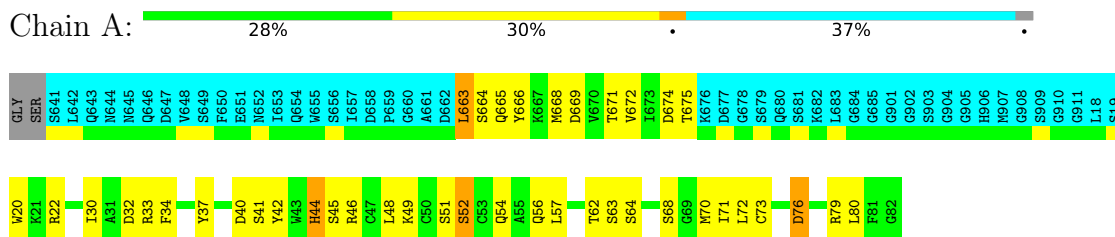
4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: DNA endonuclease RBBP8,LIM domain transcription factor LMO4



4.2.20 Score per residue for model 20

- Molecule 1: DNA endonuclease RBBP8,LIM domain transcription factor LMO4



5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure solution	1.2
ARIA	refinement	1.2

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	A	598	584	584	11±3
All	All	12000	11680	11680	225

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ALA:HB2	1:A:48:LEU:HD21	0.83	1.46	6	7
1:A:73:CYS:SG	1:A:76:ASP:HB2	0.75	2.21	15	19
1:A:30:ILE:HG23	1:A:44:HIS:HB3	0.74	1.56	4	6
1:A:664:SER:HA	1:A:667:LYS:HG3	0.74	1.58	16	1
1:A:673:ILE:HB	1:A:35:LEU:HB2	0.74	1.57	5	2
1:A:49:LYS:HA	1:A:57:LEU:HB2	0.73	1.59	13	4
1:A:44:HIS:CD2	1:A:47:CYS:HB2	0.68	2.24	9	15
1:A:670:VAL:HG11	1:A:36:LEU:HD23	0.67	1.65	9	1
1:A:25:GLY:HA3	1:A:47:CYS:SG	0.67	2.30	8	1
1:A:65:TYR:CE2	1:A:74:ARG:HG2	0.65	2.26	13	1
1:A:56:GLN:HB2	1:A:59:ASP:HB2	0.65	1.66	19	1
1:A:670:VAL:HG23	1:A:63:SER:HA	0.64	1.69	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:HD13	1:A:58:GLY:HA3	0.63	1.71	6	2
1:A:65:TYR:HE2	1:A:74:ARG:HG3	0.61	1.56	17	2
1:A:50:CYS:HB3	1:A:53:CYS:HB2	0.60	1.73	19	5
1:A:26:CYS:SG	1:A:27:GLY:N	0.60	2.72	11	2
1:A:72:LEU:HB3	1:A:76:ASP:HB3	0.59	1.75	16	2
1:A:57:LEU:HD13	1:A:64:SER:HB3	0.58	1.74	14	5
1:A:23:CYS:SG	1:A:30:ILE:HG13	0.57	2.38	11	1
1:A:57:LEU:HD21	1:A:73:CYS:HA	0.57	1.76	16	1
1:A:664:SER:HA	1:A:667:LYS:HE3	0.57	1.76	14	1
1:A:675:THR:HA	1:A:33:ARG:O	0.57	1.99	5	1
1:A:44:HIS:CD2	1:A:44:HIS:H	0.56	2.17	9	4
1:A:30:ILE:HD13	1:A:35:LEU:HB3	0.56	1.77	10	2
1:A:46:ARG:HA	1:A:56:GLN:HG2	0.56	1.75	15	1
1:A:65:TYR:HE2	1:A:74:ARG:HG2	0.56	1.57	13	2
1:A:26:CYS:SG	1:A:46:ARG:HD2	0.55	2.41	9	1
1:A:33:ARG:HG2	1:A:34:PHE:HD1	0.55	1.61	17	2
1:A:23:CYS:HB3	1:A:30:ILE:HG13	0.54	1.79	15	3
1:A:56:GLN:HB3	1:A:59:ASP:HB2	0.54	1.80	2	1
1:A:52:SER:OG	1:A:72:LEU:HG	0.54	2.03	7	3
1:A:49:LYS:HB3	1:A:56:GLN:HA	0.53	1.81	3	3
1:A:25:GLY:N	1:A:47:CYS:SG	0.53	2.80	19	6
1:A:72:LEU:HD22	1:A:80:LEU:HD13	0.53	1.81	1	1
1:A:670:VAL:HA	1:A:37:TYR:O	0.52	2.05	18	6
1:A:44:HIS:H	1:A:47:CYS:HB2	0.52	1.65	7	2
1:A:44:HIS:HD2	1:A:47:CYS:HB2	0.52	1.65	7	2
1:A:65:TYR:CE1	1:A:74:ARG:HG2	0.52	2.40	9	1
1:A:22:ARG:HA	1:A:29:LYS:HA	0.51	1.81	16	1
1:A:49:LYS:HD3	1:A:56:GLN:HA	0.51	1.81	2	1
1:A:674:ASP:HA	1:A:34:PHE:CE2	0.51	2.40	19	2
1:A:44:HIS:CD2	1:A:44:HIS:N	0.51	2.76	11	14
1:A:663:LEU:HB3	1:A:666:TYR:HD2	0.50	1.66	20	1
1:A:72:LEU:HG	1:A:76:ASP:HB3	0.50	1.83	12	1
1:A:663:LEU:HG	1:A:666:TYR:HD2	0.50	1.67	13	2
1:A:33:ARG:HG2	1:A:34:PHE:CD1	0.49	2.42	17	1
1:A:45:SER:HB3	1:A:56:GLN:HG3	0.48	1.82	4	1
1:A:667:LYS:HG3	1:A:65:TYR:CE1	0.48	2.42	19	1
1:A:32:ASP:HB2	1:A:44:HIS:HB2	0.48	1.84	20	1
1:A:57:LEU:HD23	1:A:62:THR:HB	0.48	1.84	8	1
1:A:664:SER:HA	1:A:667:LYS:HD3	0.47	1.84	11	1
1:A:32:ASP:CG	1:A:44:HIS:HB2	0.47	2.29	16	1
1:A:671:THR:HB	1:A:37:TYR:HB2	0.47	1.84	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:668:MET:SD	1:A:39:MET:HG3	0.47	2.50	15	1
1:A:52:SER:HB2	1:A:76:ASP:OD2	0.46	2.10	8	1
1:A:668:MET:SD	1:A:39:MET:HA	0.46	2.50	9	1
1:A:674:ASP:HA	1:A:34:PHE:CZ	0.46	2.46	5	2
1:A:43:TRP:HB3	1:A:47:CYS:HB3	0.46	1.88	3	3
1:A:43:TRP:CB	1:A:48:LEU:HG	0.46	2.40	18	1
1:A:673:ILE:HD13	1:A:35:LEU:HD12	0.45	1.87	15	2
1:A:30:ILE:HG12	1:A:44:HIS:CD2	0.45	2.46	7	1
1:A:21:LYS:HB3	1:A:30:ILE:HD12	0.45	1.88	2	2
1:A:38:ALA:HB2	1:A:48:LEU:HD11	0.45	1.87	4	1
1:A:65:TYR:HE1	1:A:74:ARG:HG2	0.45	1.71	9	1
1:A:20:TRP:CZ3	1:A:29:LYS:HE3	0.45	2.47	4	1
1:A:23:CYS:O	1:A:28:GLY:HA2	0.45	2.12	5	1
1:A:43:TRP:HB2	1:A:48:LEU:HG	0.45	1.88	16	3
1:A:50:CYS:HA	1:A:71:ILE:O	0.45	2.11	16	1
1:A:78:ILE:HA	1:A:82:GLY:HA2	0.44	1.87	8	2
1:A:667:LYS:HD3	1:A:63:SER:HB2	0.44	1.89	4	1
1:A:50:CYS:O	1:A:54:GLN:HA	0.44	2.12	16	6
1:A:36:LEU:HB3	1:A:48:LEU:HD12	0.44	1.88	5	1
1:A:663:LEU:HD22	1:A:77:TYR:HE2	0.44	1.73	15	1
1:A:23:CYS:HB2	1:A:28:GLY:CA	0.44	2.43	11	1
1:A:76:ASP:HA	1:A:79:ARG:HB2	0.44	1.89	7	1
1:A:663:LEU:HA	1:A:666:TYR:CD2	0.44	2.48	19	1
1:A:65:TYR:HD2	1:A:74:ARG:HA	0.43	1.72	19	1
1:A:20:TRP:CZ3	1:A:29:LYS:HB3	0.43	2.48	15	1
1:A:30:ILE:HD11	1:A:42:TYR:HB3	0.43	1.89	20	1
1:A:67:LYS:HD3	1:A:81:PHE:HB3	0.43	1.89	5	1
1:A:65:TYR:CD2	1:A:74:ARG:HA	0.43	2.48	19	1
1:A:23:CYS:HA	1:A:42:TYR:O	0.43	2.12	5	1
1:A:38:ALA:CB	1:A:48:LEU:HD21	0.43	2.44	7	1
1:A:26:CYS:N	1:A:47:CYS:SG	0.43	2.86	11	3
1:A:43:TRP:CG	1:A:48:LEU:HD23	0.43	2.49	17	1
1:A:667:LYS:HG2	1:A:65:TYR:CE1	0.42	2.48	4	1
1:A:45:SER:HB3	1:A:59:ASP:HB3	0.42	1.92	9	1
1:A:65:TYR:CE2	1:A:74:ARG:HB3	0.42	2.50	2	1
1:A:45:SER:HA	1:A:58:GLY:HA3	0.42	1.88	15	1
1:A:38:ALA:HB3	1:A:43:TRP:NE1	0.42	2.30	1	1
1:A:663:LEU:O	1:A:667:LYS:HG2	0.42	2.14	14	1
1:A:72:LEU:HD23	1:A:76:ASP:HB3	0.42	1.91	17	1
1:A:48:LEU:HD23	1:A:48:LEU:HA	0.42	1.74	18	2
1:A:65:TYR:CE2	1:A:74:ARG:HG3	0.41	2.43	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ASP:OD2	1:A:44:HIS:HB2	0.41	2.16	4	1
1:A:23:CYS:HB2	1:A:28:GLY:H	0.41	1.74	7	1
1:A:57:LEU:HA	1:A:60:ILE:HD12	0.41	1.92	18	1
1:A:667:LYS:HA	1:A:64:SER:O	0.41	2.16	6	1
1:A:71:ILE:O	1:A:72:LEU:HD13	0.41	2.15	10	1
1:A:65:TYR:HE2	1:A:74:ARG:HB3	0.41	1.76	2	1
1:A:21:LYS:HA	1:A:21:LYS:HD3	0.41	1.54	7	1
1:A:22:ARG:HA	1:A:28:GLY:O	0.41	2.16	8	1
1:A:21:LYS:HG2	1:A:35:LEU:HD13	0.41	1.93	9	2
1:A:20:TRP:CH2	1:A:29:LYS:HE2	0.41	2.51	16	1
1:A:80:LEU:HD23	1:A:81:PHE:CE2	0.40	2.50	12	1
1:A:56:GLN:NE2	1:A:59:ASP:HB2	0.40	2.30	8	1
1:A:20:TRP:HB2	1:A:21:LYS:H	0.40	1.62	15	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	A	75/123 (61%)	64±2 (85±3%)	9±2 (12±3%)	2±1 (3±1%)	7	41
All	All	1500/2460 (61%)	1275 (85%)	181 (12%)	44 (3%)	7	41

All 11 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	67	LYS	13
1	A	40	ASP	8
1	A	33	ARG	5
1	A	32	ASP	4
1	A	56	GLN	3
1	A	20	TRP	3
1	A	26	CYS	2
1	A	38	ALA	2
1	A	27	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	A	60	ILE	1
1	A	39	MET	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	A	65/99 (66%)	36±2 (55±4%)	29±2 (45±4%)	0 2
All	All	1300/1980 (66%)	714 (55%)	586 (45%)	0 2

All 57 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	64	SER	20
1	A	37	TYR	19
1	A	41	SER	19
1	A	62	THR	19
1	A	664	SER	18
1	A	675	THR	18
1	A	52	SER	18
1	A	68	SER	18
1	A	46	ARG	17
1	A	49	LYS	17
1	A	76	ASP	17
1	A	48	LEU	16
1	A	71	ILE	16
1	A	671	THR	16
1	A	63	SER	15
1	A	47	CYS	15
1	A	45	SER	14
1	A	54	GLN	14
1	A	80	LEU	14
1	A	667	LYS	14
1	A	22	ARG	14
1	A	35	LEU	14
1	A	29	LYS	11

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Mol	Chain	Res	Type	Models (Total)
1	A	21	LYS	11
1	A	33	ARG	11
1	A	20	TRP	10
1	A	44	HIS	10
1	A	51	SER	10
1	A	74	ARG	10
1	A	79	ARG	9
1	A	668	MET	8
1	A	32	ASP	8
1	A	57	LEU	8
1	A	665	GLN	8
1	A	663	LEU	8
1	A	75	ASN	8
1	A	26	CYS	8
1	A	40	ASP	8
1	A	59	ASP	7
1	A	70	MET	7
1	A	72	LEU	7
1	A	669	ASP	6
1	A	36	LEU	6
1	A	23	CYS	6
1	A	672	VAL	5
1	A	60	ILE	5
1	A	39	MET	5
1	A	56	GLN	5
1	A	67	LYS	5
1	A	674	ASP	4
1	A	42	TYR	3
1	A	670	VAL	2
1	A	43	TRP	1
1	A	66	THR	1
1	A	78	ILE	1
1	A	673	ILE	1
1	A	53	CYS	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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