Full wwPDB NMR Structure Validation Report (i)

Apr 20, 2024 – 06:15 PM EDT

PDB ID	:	2JYB
Title	:	binary hvDHFR1:folate complex
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Deposited on	:	2007-12-10

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:

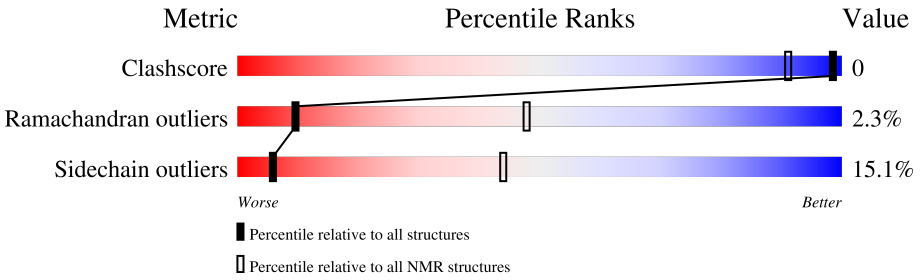
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	162	64% 15% • 19%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 18 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:1-A:10, A:27-A:65, A:71-A:122, A:129-A:158 (131)	0.44	18

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 12 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2467 atoms, of which 1202 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Dihydrofolate reductase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	162	2467	788	1202	218	255	4	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	VAL	ILE	conflict	UNP P15093

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: Dihydrofolate reductase

Chain A: 64% 15% • 19%

M1 S5 V6 A10 E11 N12 R13 V14 I15 G16 R17 D18 G19 E20 L21 P22 W23 P24 S25 I26 K30 Y33 R34 S35 R36 D40 R46 E50 R53 R66 S67 E68 R69 S70 R78 D93 A94 Y98 Y106 R115 L118 S119 R120 G123

E124 Y125 E126 G127 D128 P132 E133 W134 W139 T151 W155 V156 R157 S158 A159 S160 S161 R162

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: Dihydrofolate reductase

Chain A: 57% 21% • 19%

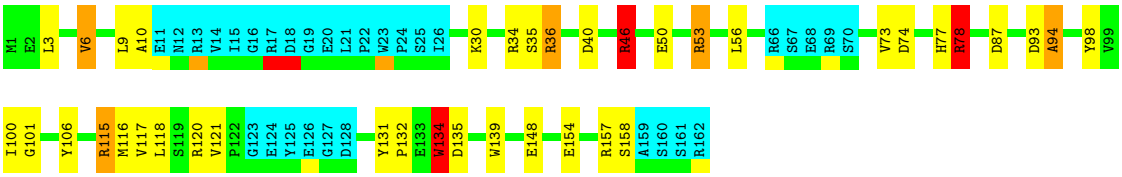
M1 S5 V6 A10 E11 N12 R13 V14 I15 G16 R17 D18 G19 E20 L21 P22 W23 P24 S25 I26 D29 K30 R34 S35 R36 D40 R46 E50 S51 M52 R53 D54 S59 R66 S67 E68 R69 S70 R78 S81 V82 E83 E84 D93 A94 Y98

Y106 F109 L113 D114 R115 M116 V117 L118 S119 R120 G123 E124 Y125 E126 G127 D128 T129 Y130 Y131 P132 E133 W134 W139 D146 T151 W155 V156 R157 S158 A159 S160 S161 R162

4.2.2 Score per residue for model 2

• Molecule 1: Dihydrofolate reductase

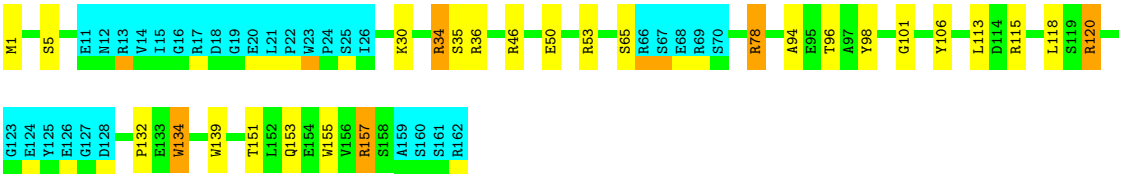
Chain A: 57% 19% • • 19%



4.2.3 Score per residue for model 3

- Molecule 1: Dihydrofolate reductase

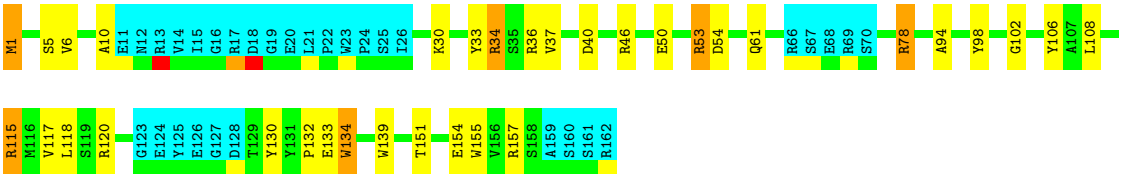
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Dihydrofolate reductase

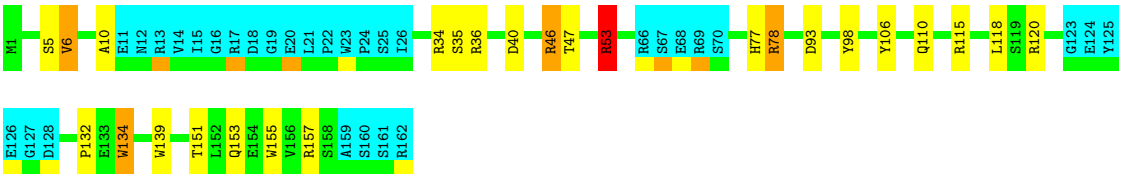
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Dihydrofolate reductase

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Dihydrofolate reductase

Chain A: 63% 16% • 19%

M1 V6 L9 A10 E11 N12 R13 V14 I15 G16 R17 D18 G19 E20 L21 P22 W23 P24 S25 I26 R34 S35 R36 D40 R46 R53 D54 D55 Q61 R66 S67 E68 R69 S70 H77 R78 D93 A94 Y98 G101 Y106 L113 D114 R115 L118

S119 R120 G123 E124 Y125 E126 G127 D128 P132 E133 W134 W139 H147 T151 R157 S158 A159 S160 S161 R162

4.2.7 Score per residue for model 7

- Molecule 1: Dihydrofolate reductase

Chain A: 63% 15% • 19%

M1 E2 S5 V6 A10 E11 N12 R13 V14 I15 G16 R17 D18 G19 E20 L21 P22 W23 P24 S25 I26 K30 Y33 R34 S35 R36 R46 R53 Q61 R66 S67 E68 R69 S70 R78 A94 Y98 G101 Y106 L113 D114 R115 M116 V117 L118 S119

R120 G123 E124 Y125 E126 G127 D128 P132 E133 W134 W139 T151 W155 V156 R157 S158 A159 S160 S161 R162

4.2.8 Score per residue for model 8

- Molecule 1: Dihydrofolate reductase

Chain A: 60% 16% 5% 19%

M1 E2 L3 V4 S5 V6 A10 E11 N12 R13 V14 I15 G16 R17 D18 G19 E20 L21 P22 W23 P24 S25 I26 K30 K31 Q32 Y33 R34 S35 R36 R46 R53 R66 S67 E68 R69 S70 V73 R78 D93 A94 E95 T96 A97 Y98 V99 I100 Y106 F109

R115 M116 V117 L118 S119 R120 G123 E124 Y125 E126 G127 D128 Y131 P132 E133 W134 W139 E148 T151 L152 Q153 E154 W155 V156 R157 S158 A159 S160 S161 R162

4.2.9 Score per residue for model 9

- Molecule 1: Dihydrofolate reductase

Chain A: 64% 12% • • 19%

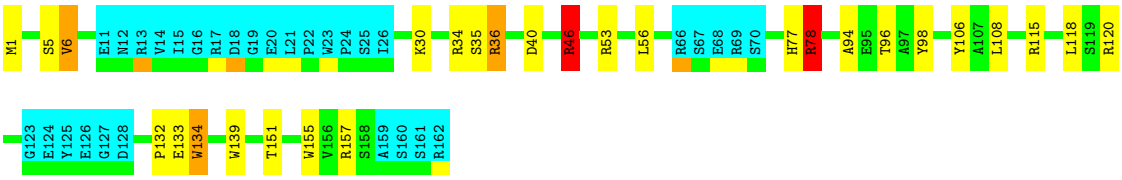
M1 S5 V6 A10 E11 N12 R13 V14 I15 G16 R17 D18 G19 E20 L21 P22 W23 P24 S25 I26 K30 Y33 R34 S35 R36 D40 R46 R53 S59 R66 S67 E68 R69 S70 R78 D87 A94 Y98 Y106 A107 L108 R115 L118 S119

R120 G123 E124 Y125 E126 G127 D128 P132 E133 W134 W139 E148 W155 V156 R157 S158 A159 S160 S161 R162

4.2.10 Score per residue for model 10

- Molecule 1: Dihydrofolate reductase

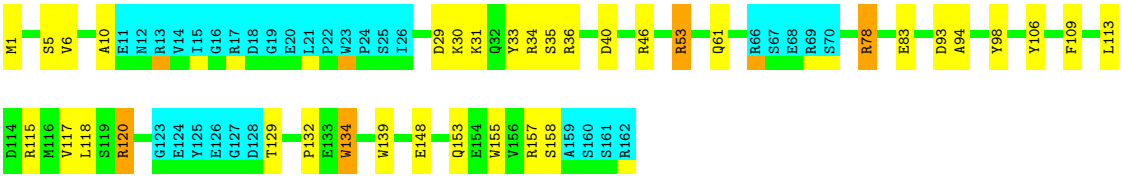
Chain A: 64% 14% • • 19%



4.2.11 Score per residue for model 11

- Molecule 1: Dihydrofolate reductase

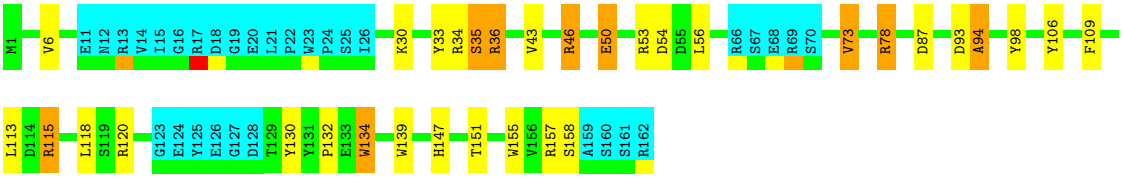
Chain A: 59% 20% • 19%



4.2.12 Score per residue for model 12

- Molecule 1: Dihydrofolate reductase

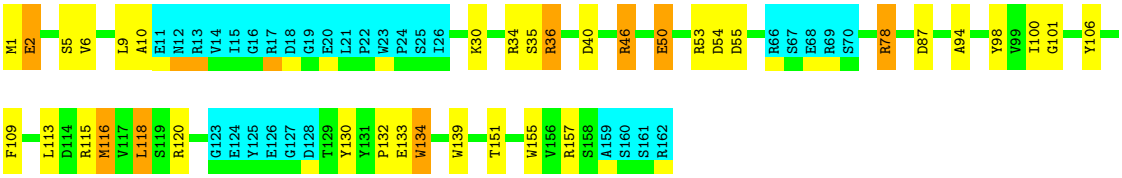
Chain A: 60% 15% 6% 19%



4.2.13 Score per residue for model 13

- Molecule 1: Dihydrofolate reductase

Chain A: 58% 18% 5% 19%



4.2.14 Score per residue for model 14

- Molecule 1: Dihydrofolate reductase

Chain A: 63% 15% • 19%

M1 V6 L9 A10 E11 N12 R13 V14 I15 G16 R17 D18 G19 E20 L21 P22 W23 P24 S25 I26 K30 Y33 R34 S35 R36 D40 R46 E50 R53 L56 S59 R66 S67 E68 R69 S70 V73 R78 E84 A94 Y98 Y106

R115 L118 S119 R120 G123 E124 Y125 E126 G127 D128 P132 E133 W134 W139 W155 V156 R157 S158 A159 S160 S161 R162

4.2.15 Score per residue for model 15

- Molecule 1: Dihydrofolate reductase

Chain A: 64% 12% • • 19%

M1 V6 E11 N12 R13 V14 I15 G16 R17 D18 G19 E20 L21 P22 W23 P24 S25 I26 K30 R34 S35 R36 R46 R53 S59 R66 S67 E68 R69 S70 R78 D93 A94 Y98 G101 Y106 L113 D114 R115 L118 S119 R120 G123 E124

Y125 E126 G127 D128 T129 Y130 Y131 P132 E133 W134 W139 E148 W155 V156 R157 S158 A159 S160 S161 R162

4.2.16 Score per residue for model 16

- Molecule 1: Dihydrofolate reductase

Chain A: 60% 15% 5% 19%

M1 S5 V6 L9 A10 E11 N12 R13 V14 I15 G16 R17 D18 G19 E20 L21 P22 W23 P24 S25 I26 P27 A28 Y33 R34 S35 R36 V43 R46 R53 S59 M64 S65 R66 S67 E68 R69 S70 R78 A94 Y98 G101 Y106 A107 L108 F109

R115 M116 V117 L118 S119 R120 G123 E124 Y125 E126 G127 D128 T129 Y130 Y131 P132 E133 W134 D135 E138 W139 T151 W155 V156 R157 S158 A159 S160 S161 R162

4.2.17 Score per residue for model 17

- Molecule 1: Dihydrofolate reductase

Chain A: 60% 17% • 19%

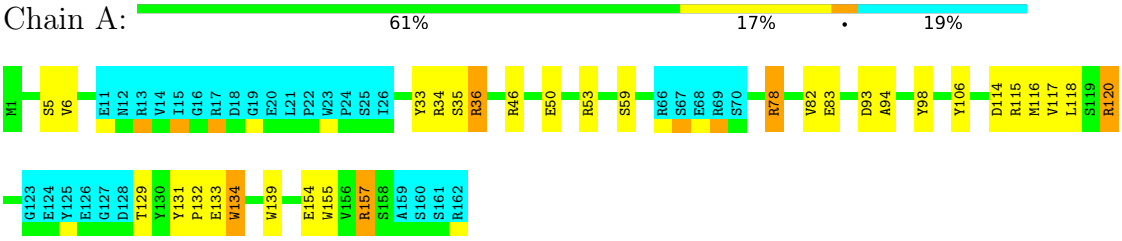
M1 S5 V6 A10 E11 N12 R13 V14 I15 G16 R17 D18 G19 E20 L21 P22 W23 P24 S25 I26 K30 Y33 R34 S35 R36 V43 R46 E50 S51 M52 R53 Q61 R66 S67 E68 R69 S70 R78 D93 A94 Y98 Y106 A107 L108 F109 R115

M116 V117 L118 S119 R120 G123 E124 Y125 E126 G127 D128 T129 Y130 Y131 P132 E133 W134 W139 T151 L152 Q153 E154 W155 V156 R157 S158 A159 S160 S161 R162

4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Dihydrofolate reductase

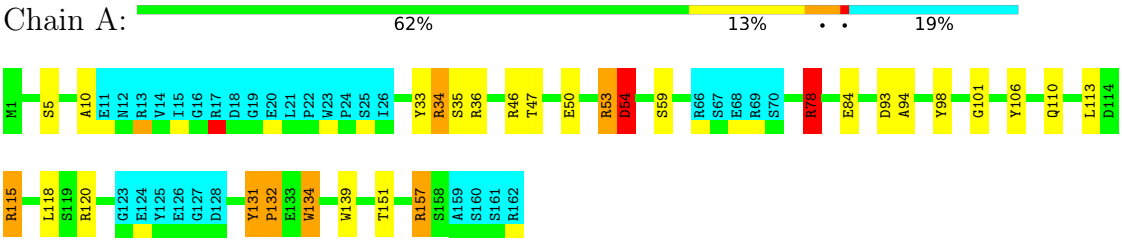
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Dihydrofolate reductase

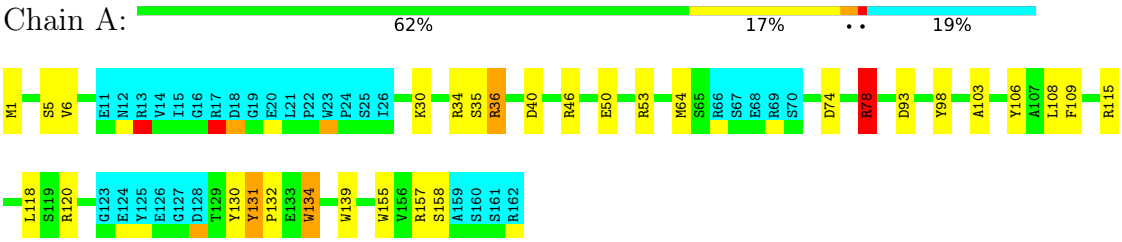
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Dihydrofolate reductase

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 100 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
CNS	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	1.32±0.01	0±0/1043 (0.0± 0.0%)	1.65±0.01	16±1/1424 (1.1± 0.1%)
All	All	1.32	0/20860 (0.0%)	1.65	321/28480 (1.1%)

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	5.5±2.2
All	All	0	111

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	36	ARG	NE-CZ-NH1	11.93	126.26	120.30	20	20
1	A	115	ARG	NE-CZ-NH1	11.92	126.26	120.30	2	20
1	A	78	ARG	NE-CZ-NH1	11.90	126.25	120.30	6	18
1	A	53	ARG	NE-CZ-NH1	10.15	125.38	120.30	17	20
1	A	120	ARG	NE-CZ-NH1	9.89	125.25	120.30	20	20
1	A	157	ARG	NE-CZ-NH1	9.27	124.93	120.30	12	18
1	A	34	ARG	NE-CZ-NH1	9.23	124.92	120.30	15	20
1	A	50	GLU	CA-CB-CG	9.01	133.22	113.40	13	1
1	A	157	ARG	NE-CZ-NH2	-8.84	115.88	120.30	12	6
1	A	115	ARG	NE-CZ-NH2	-8.70	115.95	120.30	2	7
1	A	46	ARG	NE-CZ-NH1	8.61	124.60	120.30	7	19
1	A	120	ARG	NE-CZ-NH2	-8.39	116.10	120.30	14	8
1	A	53	ARG	NE-CZ-NH2	-7.46	116.57	120.30	5	4
1	A	139	TRP	CD1-NE1-CE2	-7.39	102.35	109.00	9	20
1	A	36	ARG	NE-CZ-NH2	-7.38	116.61	120.30	20	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	46	ARG	NE-CZ-NH2	-6.99	116.81	120.30	16	7
1	A	10	ALA	N-CA-CB	-6.85	100.51	110.10	5	7
1	A	94	ALA	N-CA-CB	-6.69	100.73	110.10	12	3
1	A	78	ARG	NE-CZ-NH2	-6.69	116.96	120.30	5	4
1	A	10	ALA	CB-CA-C	6.45	119.77	110.10	4	5
1	A	33	TYR	CB-CG-CD2	-6.42	117.15	121.00	9	1
1	A	50	GLU	CB-CA-C	6.27	122.93	110.40	12	2
1	A	34	ARG	NE-CZ-NH2	-6.06	117.27	120.30	18	7
1	A	155	TRP	CD1-NE1-CE2	-6.01	103.59	109.00	12	17
1	A	6	VAL	CA-CB-CG2	5.98	119.87	110.90	12	12
1	A	134	TRP	CD1-NE1-CE2	-5.98	103.62	109.00	20	20
1	A	43	VAL	CA-CB-CG2	5.69	119.43	110.90	17	3
1	A	37	VAL	CA-CB-CG2	5.66	119.40	110.90	4	1
1	A	2	GLU	CB-CA-C	5.64	121.67	110.40	13	1
1	A	96	THR	CA-CB-CG2	5.46	120.05	112.40	10	3
1	A	101	GLY	O-C-N	-5.44	113.95	123.20	2	5
1	A	54	ASP	CB-CG-OD2	5.44	123.20	118.30	19	1
1	A	52	MET	CA-CB-CG	5.43	122.54	113.30	1	1
1	A	133	GLU	CB-CA-C	5.39	121.18	110.40	4	2
1	A	121	VAL	CA-CB-CG2	5.30	118.86	110.90	2	1
1	A	151	THR	CA-CB-CG2	5.29	119.81	112.40	8	1
1	A	73	VAL	CA-CB-CG2	5.21	118.72	110.90	14	2
1	A	117	VAL	CA-CB-CG2	5.17	118.66	110.90	11	1
1	A	131	TYR	CB-CG-CD2	-5.11	117.93	121.00	15	1
1	A	6	VAL	CA-CB-CG1	5.10	118.55	110.90	4	1
1	A	157	ARG	N-CA-CB	5.06	119.70	110.60	15	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	35	SER	Peptide	17
1	A	30	LYS	Peptide	11
1	A	50	GLU	Peptide	7
1	A	130	TYR	Sidechain	7
1	A	78	ARG	Sidechain	7
1	A	115	ARG	Sidechain	7
1	A	34	ARG	Peptide,Sidechain	6
1	A	53	ARG	Sidechain	5
1	A	9	LEU	Peptide	4

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	77	HIS	Sidechain	4
1	A	46	ARG	Sidechain	3
1	A	131	TYR	Sidechain	3
1	A	101	GLY	Peptide	3
1	A	157	ARG	Sidechain	3
1	A	33	TYR	Sidechain	3
1	A	1	MET	Peptide	2
1	A	147	HIS	Sidechain	2
1	A	100	ILE	Peptide	2
1	A	106	TYR	Sidechain	2
1	A	120	ARG	Sidechain	2
1	A	36	ARG	Sidechain	2
1	A	134	TRP	Peptide	1
1	A	148	GLU	Peptide	1
1	A	109	PHE	Sidechain	1
1	A	28	ALA	Peptide	1
1	A	138	GLU	Peptide	1
1	A	82	VAL	Peptide	1
1	A	54	ASP	Peptide	1
1	A	103	ALA	Peptide	1

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	1019	976	973	0±1
All	All	20380	19520	19460	5

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:116:MET:SD	1:A:118:LEU:HD12	0.54	2.41	13	1
1:A:117:VAL:HG12	1:A:154:GLU:CG	0.54	2.33	4	2
1:A:117:VAL:HG12	1:A:154:GLU:HG2	0.42	1.91	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:73:VAL:HG12	1:A:74:ASP:H	0.42	1.75	2	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	130/162 (80%)	105±3 (81±3%)	22±3 (17±3%)	3±1 (2±1%)	9	48
All	All	2600/3240 (80%)	2107 (81%)	433 (17%)	60 (2%)	9	48

All 13 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	132	PRO	20
1	A	94	ALA	18
1	A	93	ASP	6
1	A	158	SER	5
1	A	73	VAL	2
1	A	148	GLU	2
1	A	102	GLY	1
1	A	30	LYS	1
1	A	46	ARG	1
1	A	35	SER	1
1	A	157	ARG	1
1	A	52	MET	1
1	A	83	GLU	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	106/132 (80%)	90±3 (85±3%)	16±3 (15±3%)	6 44
All	All	2120/2640 (80%)	1799 (85%)	321 (15%)	6 44

All 56 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	98	TYR	20
1	A	106	TYR	20
1	A	118	LEU	20
1	A	78	ARG	19
1	A	134	TRP	18
1	A	5	SER	15
1	A	6	VAL	12
1	A	151	THR	12
1	A	40	ASP	11
1	A	113	LEU	9
1	A	133	GLU	9
1	A	36	ARG	9
1	A	1	MET	9
1	A	46	ARG	8
1	A	116	MET	8
1	A	59	SER	7
1	A	109	PHE	7
1	A	157	ARG	7
1	A	33	TYR	7
1	A	93	ASP	6
1	A	108	LEU	6
1	A	54	ASP	5
1	A	153	GLN	5
1	A	61	GLN	5
1	A	56	LEU	4
1	A	87	ASP	4
1	A	50	GLU	4
1	A	53	ARG	4
1	A	131	TYR	4
1	A	30	LYS	3
1	A	84	GLU	3
1	A	120	ARG	3
1	A	129	THR	3
1	A	29	ASP	2
1	A	83	GLU	2
1	A	3	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	135	ASP	2
1	A	47	THR	2
1	A	110	GLN	2
1	A	55	ASP	2
1	A	2	GLU	2
1	A	34	ARG	2
1	A	148	GLU	2
1	A	43	VAL	2
1	A	64	MET	2
1	A	81	SER	1
1	A	146	ASP	1
1	A	100	ILE	1
1	A	65	SER	1
1	A	32	GLN	1
1	A	31	LYS	1
1	A	9	LEU	1
1	A	114	ASP	1
1	A	115	ARG	1
1	A	132	PRO	1
1	A	74	ASP	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)

No chemical shift data were provided