Full wwPDB NMR Structure Validation Report (i)

Mar 6, 2022 – 11:33 AM EST

PDB ID	:	2KJ4
Title	:	Solution structure of the complex of VEK-30 and plasminogen kringle 2
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Deposited on	:	2009-05-21

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 following versions of software and data (see references (i)) were used in the production of this report:

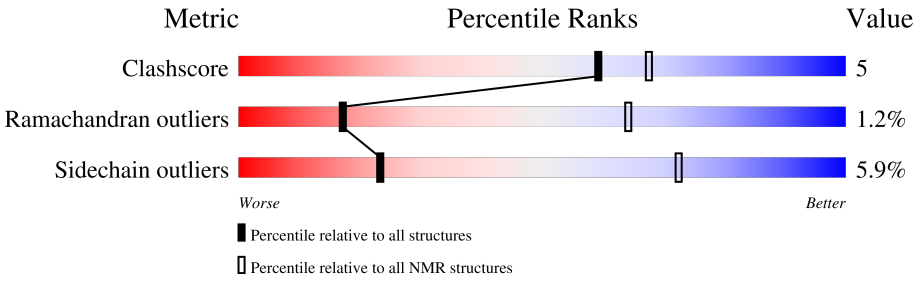
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	87	70% 10% 20%
2	B	32	31% 12% 56%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 6 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:13-A:82, B:108-B:121 (84)	0.31	6

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1891 atoms, of which 915 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called plasminogen.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	87	1364	442	653	126	135	8	0

- Molecule 2 is a protein called VEK-30.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	32	527	160	262	48	57	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	99	GLY	-	expression tag	UNP Q6V4L8
B	100	SER	-	expression tag	UNP Q6V4L8
B	130	TYR	-	insertion	UNP Q6V4L8

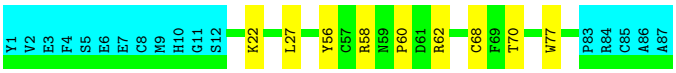
4 Residue-property plots (i)

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: plasminogen

Chain A: 70% 10% 20%



• Molecule 2: VEK-30

Chain B: 31% 12% 56%

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: plasminogen

Chain A: 63% 16% • 20%

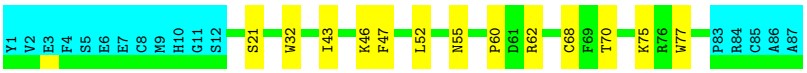
• Molecule 2: VEK-30

Chain B: 38% 6% 56%

4.2.2 Score per residue for model 2

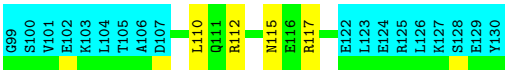
- Molecule 1: plasminogen

Chain A: 66% 15% 20%



- Molecule 2: VEK-30

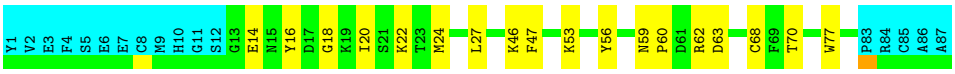
Chain B: 31% 12% 56%



4.2.3 Score per residue for model 3

- Molecule 1: plasminogen

Chain A: 60% 21% 20%



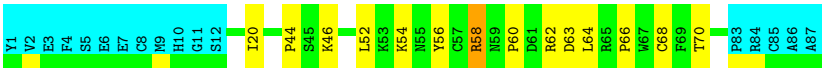
- Molecule 2: VEK-30

Chain B: 31% 12% 56%

4.2.4 Score per residue for model 4

- Molecule 1: plasminogen

Chain A: 64% 15% • 20%



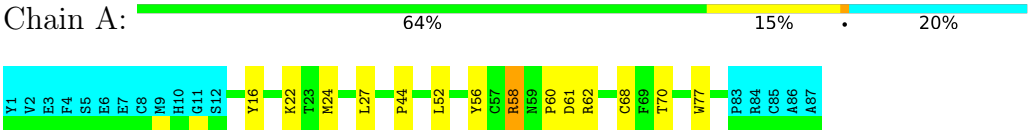
- Molecule 2: VEK-30

Chain B: 25% 16% • 56%

4.2.5 Score per residue for model 5

- Molecule 1: plasminogen

Chain A:



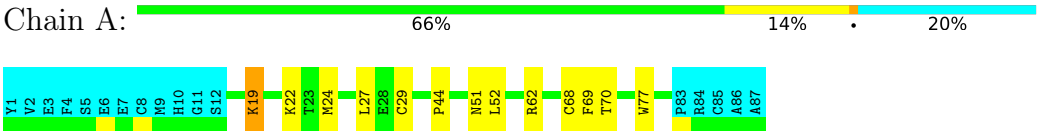
- Molecule 2: VEK-30

Chain B:

4.2.6 Score per residue for model 6 (medoid)

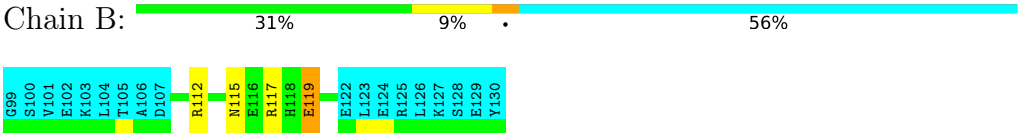
- Molecule 1: plasminogen

Chain A:



- Molecule 2: VEK-30

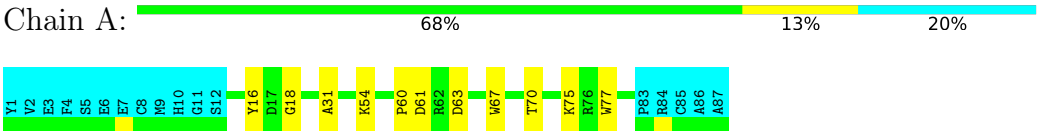
Chain B:



4.2.7 Score per residue for model 7

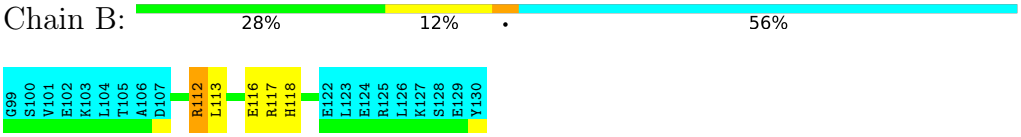
- Molecule 1: plasminogen

Chain A:



- Molecule 2: VEK-30

Chain B:



4.2.8 Score per residue for model 8

- Molecule 1: plasminogen

Chain A: 62% 18% 20%

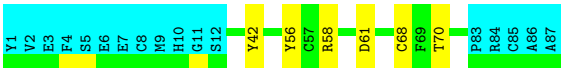
- Molecule 2: VEK-30

Chain B: 34% 6% • 56%

4.2.9 Score per residue for model 9

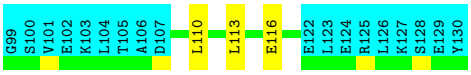
- Molecule 1: plasminogen

Chain A: 74% 7% 20%



- Molecule 2: VEK-30

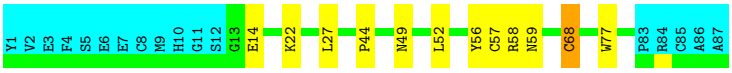
Chain B: 34% 9% 56%



4.2.10 Score per residue for model 10

- Molecule 1: plasminogen

Chain A: 67% 13% • 20%



- Molecule 2: VEK-30

Chain B: 38% 6% 56%

4.2.11 Score per residue for model 11

- Molecule 1: plasminogen

Chain A: 62% 17% • 20%

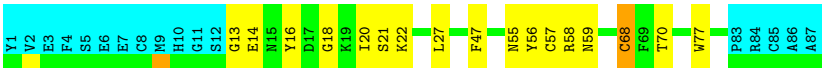
- Molecule 2: VEK-30

Chain B: 38% 6% 56%

4.2.12 Score per residue for model 12

- Molecule 1: plasminogen

Chain A: 61% 18% • 20%



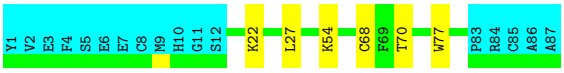
- Molecule 2: VEK-30

Chain B: 34% 9% 56%

4.2.13 Score per residue for model 13

- Molecule 1: plasminogen

Chain A: 74% 7% 20%



- Molecule 2: VEK-30

Chain B: 38% 6% 56%

4.2.14 Score per residue for model 14

- Molecule 1: plasminogen

Chain A: 63% 11% 6% 20%

Y1 V2 E3 F4 S5 E6 E7 C8 M9 H10 G11 S12 Y16 D17 G18 K19 I43 P44 S45 K46 K50 N51 L52 Y56 C57 R58 N59 P60 P66 W67 C68 F69 T70 W77 P83 R84 C85 A86 A87

- Molecule 2: VEK-30

Chain B: 25% 16% • 56%

G99 S100 V101 E102 K103 L104 T105 A106 D107 R112 L113 K114 N115 E116 R117 H118 E119 E122 L123 E124 R125 L126 K127 S128 E129 Y130

4.2.15 Score per residue for model 15

- Molecule 1: plasminogen

Chain A: 67% 13% • 20%

Y1 V2 E3 F4 S5 E6 E7 C8 M9 H10 G11 S12 G13 E14 I20 S21 H40 N55 Y56 P60 D61 R62 P66 W67 C68 F69 T70 W77 P83 R84 C85 A86 A87

- Molecule 2: VEK-30

Chain B: 31% 12% 56%

G99 S100 V101 E102 K103 L104 T105 A106 D107 R112 N115 E116 R117 H118 E119 E122 L123 E124 R125 L126 K127 S128 E129 Y130

4.2.16 Score per residue for model 16

- Molecule 1: plasminogen

Chain A: 70% 10% 20%

Y1 V2 E3 F4 S5 E6 E7 C8 M9 H10 G11 S12 G13 E14 M24 Q35 H40 K46 N59 R62 C68 F69 T70 P83 R84 C85 A86 A87

- Molecule 2: VEK-30

Chain B: 34% 9% 56%

G99 S100 V101 E102 K103 L104 T105 A106 D107 A108 E109 R112 N115 E122 L123 E124 R125 L126 K127 S128 E129 Y130

4.2.17 Score per residue for model 17

- Molecule 1: plasminogen

Chain A: 66% 14% • 20%

Y1 V2 E3 F4 S5 E6 E7 C8 M9 H10 G11 S12 Y16 I20 Q30 H38 I43 K46 F47 P60 D61 R62 P66 W67 C68 F69 T70 W77 P83 R84 C85 A86 A87

- Molecule 2: VEK-30

Chain B: 31% 9% • 56%

G99 S100 V101 E102 K103 L104 T105 A106 D107 L110 N115 E116 R117 H118 E119 E122 L123 E124 R125 L126 K127 S128 E129 Y130

4.2.18 Score per residue for model 18

- Molecule 1: plasminogen

Chain A: 63% 17% 20%

Y1 V2 E3 F4 S5 E6 E7 C8 M9 H10 G11 S12 G13 K19 I20 S21 H40 G41 Y42 Y56 C57 R58 N59 P60 R65 P66 W67 C68 F69 T70 W77 C80 D81 I82 P83 R84 C85 A86 A87

- Molecule 2: VEK-30

Chain B: 31% 12% 56%

G99 S100 V101 E102 K103 L104 T105 A106 D107 E116 R117 H118 E119 E120 A121 E122 L123 E124 R125 L126 K127 S128 E129 Y130

4.2.19 Score per residue for model 19

- Molecule 1: plasminogen

Chain A: 69% 11% 20%

Y1 V2 E3 F4 S5 E6 E7 C8 M9 H10 G11 S12 N15 S21 K22 L27 H40 K53 K54 N55 C68 F69 T70 W77 P83 R84 C85 A86 A87

- Molecule 2: VEK-30

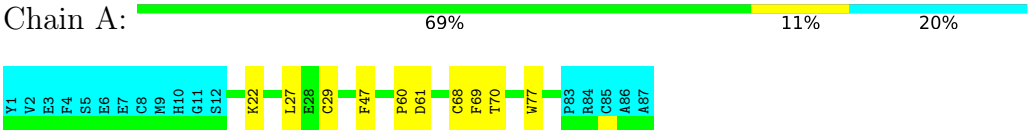
Chain B: 31% 12% 56%

G99 S100 V101 E102 K103 L104 T105 A106 D107 K114 N115 E116 R117 H118 E119 E122 L123 E124 R125 L126 K127 S128 E129 Y130

4.2.20 Score per residue for model 20

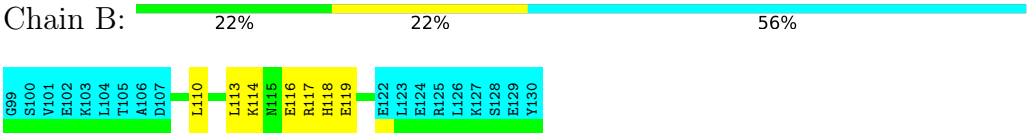
- Molecule 1: plasminogen

Chain A:



- Molecule 2: VEK-30

Chain B:



5 Refinement protocol and experimental data overview (i)

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

Of the 50 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	structure solution	1.1
CNS	refinement	1.1

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	0.82±0.02	0±0/599 (0.0± 0.0%)	0.70±0.02	0±0/813 (0.0± 0.0%)
2	B	0.75±0.06	0±0/121 (0.0± 0.0%)	0.76±0.07	0±0/161 (0.0± 0.1%)
All	All	0.81	0/14400 (0.0%)	0.71	2/19480 (0.0%)

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	0.1±0.4
All	All	0	3

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	46	LYS	N-CA-CB	-5.23	101.18	110.60	16	1
2	B	117	ARG	NE-CZ-NH2	-5.00	117.80	120.30	17	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	62	ARG	Sidechain	1
1	A	76	ARG	Sidechain	1
1	A	58	ARG	Sidechain	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	579	538	536	5±2
2	B	120	117	116	2±1
All	All	13980	13100	13040	129

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:TYR:HB2	1:A:58:ARG:NH1	0.69	2.02	5	6
1:A:21:SER:HB2	1:A:55:ASN:ND2	0.62	2.09	11	5
2:B:113:LEU:HB3	2:B:117:ARG:NH2	0.60	2.12	4	3
1:A:14:GLU:HA	1:A:59:ASN:O	0.56	2.01	3	3
1:A:47:PHE:CE1	2:B:110:LEU:HB3	0.55	2.36	17	4
1:A:22:LYS:HA	1:A:27:LEU:O	0.53	2.04	5	11
1:A:77:TRP:NE1	2:B:117:ARG:HB3	0.53	2.17	1	17
1:A:44:PRO:HB3	1:A:52:LEU:O	0.53	2.03	14	5
1:A:56:TYR:O	1:A:58:ARG:HG2	0.51	2.04	14	3
1:A:47:PHE:CE1	2:B:110:LEU:HB2	0.51	2.41	20	1
1:A:19:LYS:H	1:A:19:LYS:HD3	0.51	1.66	14	2
1:A:61:ASP:HA	2:B:110:LEU:CD1	0.51	2.36	20	1
2:B:112:ARG:HA	2:B:115:ASN:ND2	0.51	2.21	2	6
1:A:42:TYR:OH	1:A:61:ASP:HB3	0.51	2.06	9	1
2:B:114:LYS:HG2	2:B:118:HIS:CE1	0.50	2.42	14	1
1:A:57:CYS:O	1:A:58:ARG:HD3	0.50	2.07	12	2
1:A:29:CYS:HA	1:A:69:PHE:O	0.49	2.08	20	2
1:A:47:PHE:CZ	2:B:110:LEU:HB3	0.49	2.42	12	1
1:A:20:ILE:O	1:A:56:TYR:HA	0.49	2.08	4	3
1:A:35:GLN:NE2	1:A:40:HIS:H	0.48	2.04	16	1
1:A:30:GLN:OE1	1:A:38:HIS:HB2	0.48	2.08	11	1
2:B:112:ARG:NH2	2:B:116:GLU:HB2	0.48	2.23	7	1
2:B:112:ARG:O	2:B:112:ARG:HD3	0.48	2.09	5	1
2:B:113:LEU:O	2:B:116:GLU:HB3	0.48	2.09	7	4
1:A:43:ILE:O	1:A:46:LYS:HG2	0.47	2.08	8	5
1:A:61:ASP:HA	2:B:110:LEU:HD11	0.47	1.84	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:LYS:HE2	1:A:50:LYS:HA	0.47	1.87	1	1
1:A:68:CYS:HB2	1:A:80:CYS:SG	0.46	2.51	11	1
1:A:14:GLU:HG2	1:A:59:ASN:O	0.46	2.10	10	1
2:B:115:ASN:O	2:B:119:GLU:HG2	0.46	2.11	17	1
1:A:16:TYR:OH	1:A:20:ILE:HB	0.45	2.11	12	2
1:A:50:LYS:CG	1:A:60:PRO:HA	0.45	2.42	14	1
1:A:75:LYS:HD2	1:A:77:TRP:O	0.45	2.10	7	1
1:A:61:ASP:O	1:A:62:ARG:HB2	0.45	2.12	5	1
1:A:63:ASP:CG	1:A:64:LEU:H	0.44	2.16	4	1
1:A:63:ASP:OD1	2:B:118:HIS:NE2	0.44	2.51	7	1
1:A:61:ASP:HB2	2:B:114:LYS:HB2	0.44	1.90	20	1
1:A:13:GLY:HA3	1:A:66:PRO:HG3	0.44	1.90	11	2
1:A:16:TYR:CZ	1:A:18:GLY:HA3	0.44	2.47	7	4
2:B:116:GLU:O	2:B:120:GLU:HG2	0.43	2.13	18	1
1:A:30:GLN:OE1	1:A:38:HIS:HB3	0.43	2.14	17	1
1:A:61:ASP:HA	2:B:110:LEU:HD13	0.43	1.90	9	1
1:A:21:SER:HB3	1:A:55:ASN:ND2	0.42	2.29	12	1
1:A:31:ALA:HA	1:A:54:LYS:O	0.42	2.14	7	1
1:A:58:ARG:HH11	1:A:58:ARG:HG2	0.42	1.74	12	1
1:A:61:ASP:OD2	1:A:67:TRP:HZ2	0.42	1.98	7	1
1:A:54:LYS:HA	1:A:54:LYS:HE2	0.42	1.92	4	1
1:A:65:ARG:HD3	1:A:80:CYS:O	0.42	2.15	18	1
1:A:70:THR:HB	1:A:75:LYS:O	0.41	2.16	1	1
2:B:114:LYS:HG3	2:B:117:ARG:NH2	0.41	2.30	19	2
1:A:14:GLU:OE2	1:A:62:ARG:HG3	0.41	2.16	15	1
1:A:40:HIS:CD2	1:A:42:TYR:HB2	0.41	2.51	18	1
1:A:57:CYS:HA	1:A:68:CYS:SG	0.41	2.56	12	2
1:A:13:GLY:HA3	1:A:66:PRO:CG	0.40	2.46	11	1
1:A:32:TRP:CG	1:A:52:LEU:HG	0.40	2.50	2	1
1:A:51:ASN:HB3	1:A:58:ARG:HH21	0.40	1.75	8	1
1:A:40:HIS:HD2	1:A:42:TYR:HB2	0.40	1.77	18	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	70/87 (80%)	64±2 (92±2%)	5±2 (7±2%)	1±1 (1±1%)	15	61
2	B	14/32 (44%)	14±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	1680/2380 (71%)	1566 (93%)	94 (6%)	20 (1%)	17	64

All 5 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	60	PRO	13
1	A	62	ARG	4
1	A	63	ASP	1
1	A	54	LYS	1
1	A	52	LEU	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	64/78 (82%)	61±1 (95±2%)	3±1 (5±2%)	26	75
2	B	12/28 (43%)	11±1 (91±7%)	1±1 (9±7%)	13	60
All	All	1520/2120 (72%)	1431 (94%)	89 (6%)	23	72

All 21 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	68	CYS	19
1	A	70	THR	18
2	B	119	GLU	9
1	A	24	MET	6
2	B	112	ARG	6
1	A	19	LYS	5
2	B	115	ASN	5
1	A	62	ARG	4
1	A	46	LYS	2
1	A	53	LYS	2
1	A	58	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	40	HIS	2
1	A	78	GLU	1
1	A	75	LYS	1
2	B	118	HIS	1
1	A	51	ASN	1
1	A	49	ASN	1
1	A	35	GLN	1
1	A	50	LYS	1
1	A	21	SER	1
1	A	15	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 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