Full wwPDB NMR Structure Validation Report (i)

Oct 23, 2021 – 05:40 PM EDT

PDB ID	:	1QFN
Title	:	GLUTAREDOXIN-1-RIBONUCLEOTIDE REDUCTASE B1 MIXED DISULFIDE BOND
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Deposited on	:	1999-04-12

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:

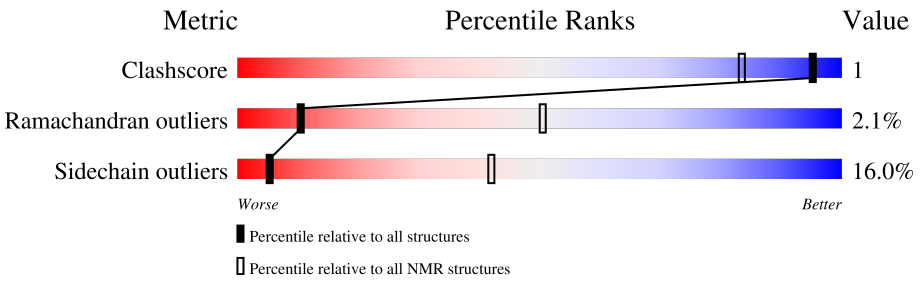
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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	85	82% 18%
2	B	25	28% 72%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:85, B:144-B:150 (92)	0.39	14

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 5 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1670 atoms, of which 813 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (GLUTAREDOXIN 1).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	85	1340	429	658	116	135	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	SER	CYS	engineered mutation	UNP P68688

- Molecule 2 is a protein called PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	25	330	101	155	28	45	1	0

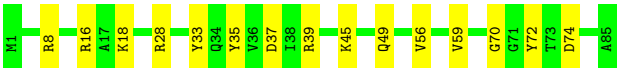
4 Residue-property plots (i)

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: PROTEIN (GLUTAREDOXIN 1)

Chain A: 82% 18%



• Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

Chain B: 28% 72%

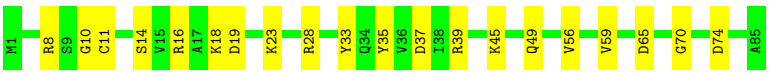
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

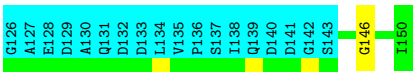
• Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A: 76% 24%



• Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

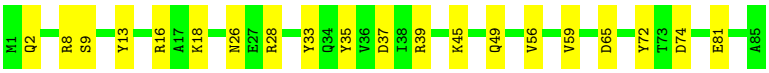
Chain B: 24% • 72%



4.2.2 Score per residue for model 2

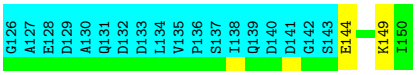
• Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A: 76% 24%



• Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

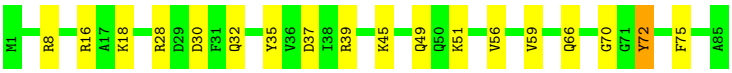
Chain B: 20% 8% 72%



4.2.3 Score per residue for model 3

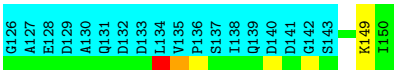
• Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A: 79% 20% •



• Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

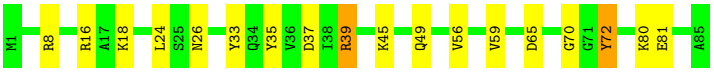
Chain B: 24% • 72%



4.2.4 Score per residue for model 4

• Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A: 79% 19% •



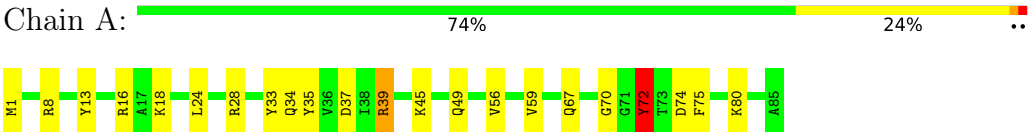
• Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

Chain B: 20% 8% 72%

4.2.5 Score per residue for model 5

- Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A:



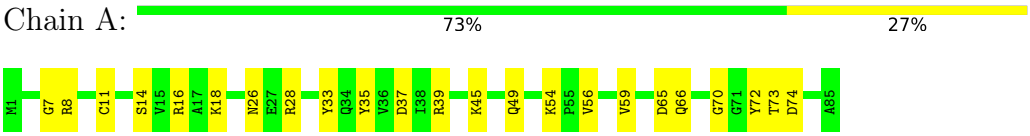
- Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

Chain B:

4.2.6 Score per residue for model 6

- Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A:



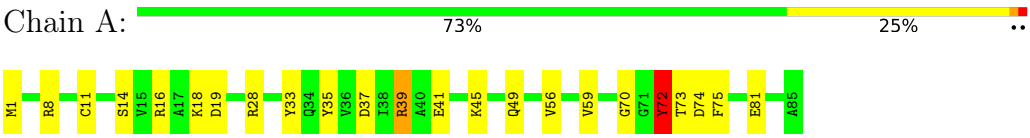
- Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

Chain B:

4.2.7 Score per residue for model 7

- Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A:



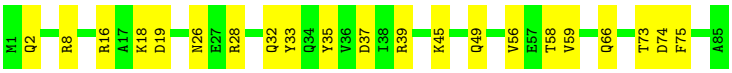
- Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

Chain B:

4.2.8 Score per residue for model 8

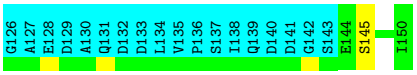
- Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A: 75% 25%



- Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

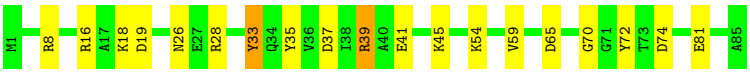
Chain B: 24% • 72%



4.2.9 Score per residue for model 9

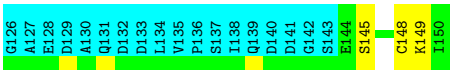
- Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A: 78% 20% •



- Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

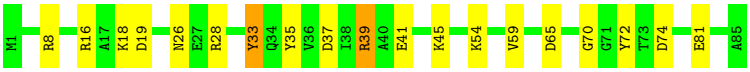
Chain B: 16% 12% 72%



4.2.10 Score per residue for model 10

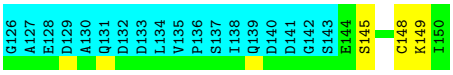
- Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A: 78% 20% •



- Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

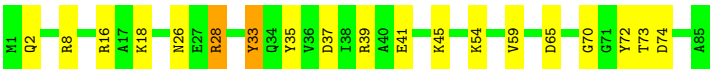
Chain B: 16% 12% 72%



4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A: 78% 20% •



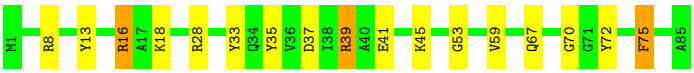
- Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

Chain B: 24% • 72%

4.2.12 Score per residue for model 12

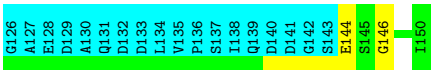
- Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A: 80% 16% •



- Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

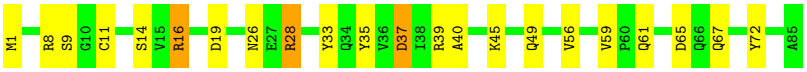
Chain B: 20% 8% 72%



4.2.13 Score per residue for model 13

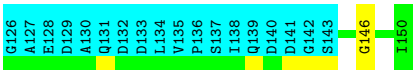
- Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A: 74% 22% •



- Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

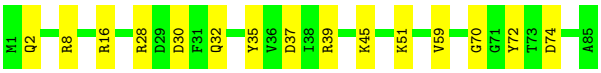
Chain B: 24% • 72%



4.2.14 Score per residue for model 14 (medoid)

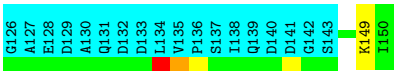
• Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A: 82% 18%



• Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

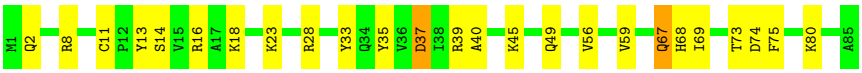
Chain B: 24% • 72%



4.2.15 Score per residue for model 15

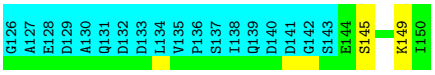
• Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A: 71% 27% •



• Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

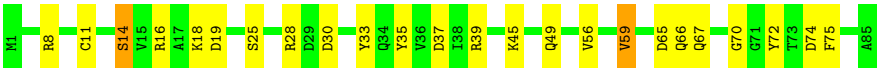
Chain B: 20% 8% 72%



4.2.16 Score per residue for model 16

• Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A: 72% 26% •



• Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

Chain B: 28% 72%

4.2.17 Score per residue for model 17

- Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A: 74% 25% •

M1 Q2 R8 C11 S14 V15 R16 A17 K18 D19 R28 D29 Y33 D37 I38 R39 K45 Q49 Q50 K51 V56 V59 G70 G71 Y72 F75 K80 A85

- Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

Chain B: 20% 8% 72%

G126 A127 E128 D129 A130 Q131 D132 D133 L134 V135 P136 S137 I138 Q139 D140 D141 G142 S143 E144 K149 I150

4.2.18 Score per residue for model 18

- Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A: 78% 18% 5%

M1 Q2 R8 S9 G10 R16 L24 R28 D29 D30 Y33 Q34 Y35 V36 D37 I38 R39 A40 K45 Q49 V59 Q66 Y72 E81 A85

- Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

Chain B: 24% • 72%

G126 A127 E128 D129 A130 Q131 D132 D133 L134 V135 P136 S137 I138 Q139 D140 D141 G142 S143 K149 I150

4.2.19 Score per residue for model 19

- Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A: 79% 19% •

M1 R8 R16 A17 K18 D19 N26 E27 R28 Y33 Q34 Y35 V36 D37 I38 R39 K45 Q49 V56 V59 G70 G71 Y72 E81 A85

- Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

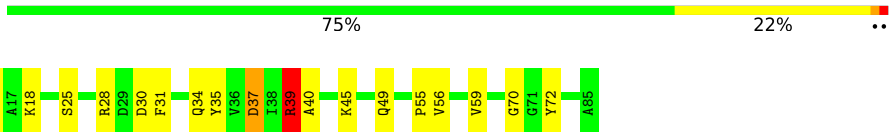
Chain B: 24% • 72%

G126 A127 E128 D129 A130 Q131 D132 D133 L134 V135 P136 S137 I138 Q139 D140 D141 G142 S143 E144 S145 I150

4.2.20 Score per residue for model 20

- Molecule 1: PROTEIN (GLUTAREDOXIN 1)

Chain A:



- Molecule 2: PROTEIN (RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1)

Chain B:

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *RESTRICTED TORSIONAL ANGLE DYNAMICS*.

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *LEAST TARGET FUNCTION*.

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

Software name	Classification	Version
OPAL	refinement	V2.6
DYANA	structure solution	

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	1.00±0.02	0±0/695 (0.0± 0.0%)	1.43±0.04	6±1/937 (0.7± 0.1%)
2	B	0.95±0.06	0±0/47 (0.0± 0.0%)	1.48±0.14	0±0/59 (0.1± 0.4%)
All	All	1.00	0/14840 (0.0%)	1.43	124/19920 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.9±1.0
All	All	0	39

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	28	ARG	NE-CZ-NH1	12.50	126.55	120.30	8	19
1	A	39	ARG	NE-CZ-NH1	12.38	126.49	120.30	1	20
1	A	16	ARG	NE-CZ-NH1	11.22	125.91	120.30	14	20
1	A	8	ARG	NE-CZ-NH1	10.26	125.43	120.30	1	20
1	A	72	TYR	CB-CG-CD2	-7.91	116.26	121.00	19	8
1	A	28	ARG	NE-CZ-NH2	-7.59	116.50	120.30	1	4
1	A	13	TYR	CB-CG-CD2	-7.54	116.48	121.00	5	2
1	A	39	ARG	CD-NE-CZ	7.08	133.50	123.60	1	5
1	A	8	ARG	NH1-CZ-NH2	-6.34	112.43	119.40	1	4
1	A	28	ARG	NH1-CZ-NH2	-5.96	112.84	119.40	16	4
1	A	39	ARG	NH1-CZ-NH2	-5.95	112.86	119.40	20	2
2	B	148	CYS	C-N-CA	5.80	136.20	121.70	6	1
1	A	8	ARG	CD-NE-CZ	5.72	131.60	123.60	20	2
1	A	13	TYR	CB-CG-CD1	5.50	124.30	121.00	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	16	ARG	CD-NE-CZ	5.30	131.02	123.60	18	2
1	A	28	ARG	CD-NE-CZ	5.29	131.01	123.60	9	3
1	A	16	ARG	NH1-CZ-NH2	-5.29	113.58	119.40	14	4
1	A	65	ASP	C-N-CA	5.06	134.35	121.70	16	1
1	A	72	TYR	CB-CG-CD1	5.03	124.02	121.00	17	1
1	A	75	PHE	CB-CG-CD2	-5.02	117.29	120.80	12	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	TYR	Sidechain	19
1	A	72	TYR	Sidechain	8
1	A	39	ARG	Sidechain	5
1	A	33	TYR	Sidechain	4
1	A	28	ARG	Sidechain	1
1	A	16	ARG	Sidechain	1
1	A	13	TYR	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	682	658	657	1±1
2	B	48	47	47	0±0
All	All	14600	14100	14080	28

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:GLN:HB3	1:A:56:VAL:HG22	0.68	1.66	19	14
1:A:11:CYS:SG	1:A:14:SER:HB2	0.52	2.45	17	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:ASP:HB2	1:A:40:ALA:HB3	0.49	1.85	13	4
1:A:56:VAL:HG21	1:A:61:GLN:NE2	0.47	2.25	13	1
1:A:67:GLN:HE22	1:A:69:ILE:HD11	0.47	1.70	15	1
1:A:11:CYS:SG	1:A:59:VAL:HG21	0.46	2.50	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	A	83/85 (98%)	72±2 (87±2%)	9±2 (11±2%)	2±1 (2±1%)	12	54
2	B	6/25 (24%)	3±1 (58±13%)	2±1 (37±16%)	0±0 (6±8%)	3	21
All	All	1780/2200 (81%)	1517 (85%)	226 (13%)	37 (2%)	10	50

All 10 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	70	GLY	15
2	B	146	GLY	5
1	A	72	TYR	4
1	A	9	SER	3
1	A	66	GLN	3
1	A	10	GLY	2
2	B	149	LYS	2
1	A	7	GLY	1
1	A	53	GLY	1
1	A	55	PRO	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	72/72 (100%)	61±2 (84±3%)	11±2 (16±3%)	5	43
2	B	5/19 (26%)	4±1 (79±18%)	1±1 (21±18%)	3	32
All	All	1540/1820 (85%)	1294 (84%)	246 (16%)	5	42

All 42 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	37	ASP	20
1	A	45	LYS	20
1	A	59	VAL	20
1	A	18	LYS	17
1	A	33	TYR	17
1	A	74	ASP	12
1	A	19	ASP	9
1	A	26	ASN	9
1	A	65	ASP	8
1	A	2	GLN	8
2	B	149	LYS	8
1	A	75	PHE	8
1	A	81	GLU	7
2	B	144	GLU	5
1	A	30	ASP	5
1	A	1	MET	5
1	A	67	GLN	5
1	A	73	THR	5
1	A	41	GLU	5
2	B	145	SER	5
1	A	72	TYR	4
1	A	80	LYS	4
1	A	39	ARG	4
1	A	54	LYS	4
1	A	32	GLN	3
1	A	51	LYS	3
1	A	24	LEU	3
1	A	34	GLN	3
2	B	148	CYS	3
1	A	23	LYS	2
1	A	66	GLN	2
1	A	28	ARG	2
1	A	25	SER	2
1	A	58	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	13	TYR	1
1	A	16	ARG	1
1	A	68	HIS	1
1	A	14	SER	1
1	A	29	ASP	1
1	A	8	ARG	1
1	A	49	GLN	1
1	A	31	PHE	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