



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 11:23 PM BST

PDB ID : 2KQE
Title : Second PBZ domain of human APLF protein in complex with ribofuranosyladenosine
Authors : Neuhaus, D.; Eustermann, S.; Brockmann, C.; Yang, J.
Deposited on : 2009-11-04

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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

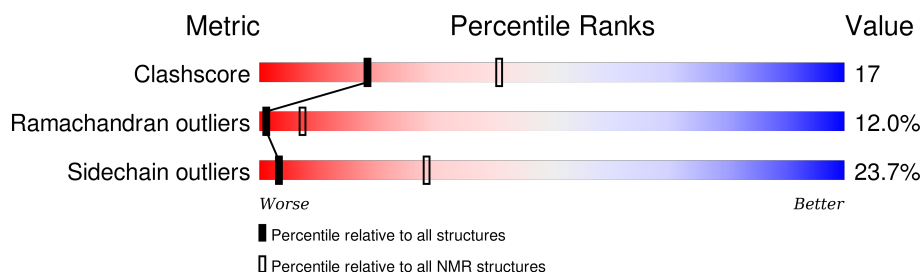
1 Overall quality at a glance

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	89	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
4	A	RIB	1003	1	-

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 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:416-A:451 (36)	1.18	4

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 1 single-model cluster was found.

Cluster number	Models
1	1, 4, 5, 7, 8, 9, 10
2	2, 6
Single-model clusters	3

3 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 786 atoms, of which 376 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Aprataxin and PNK-like factor.

Mol	Chain	Residues	Atoms						Trace
1	A	47	Total	C	H	N	O	S	0
			736	232	355	71	76	2	

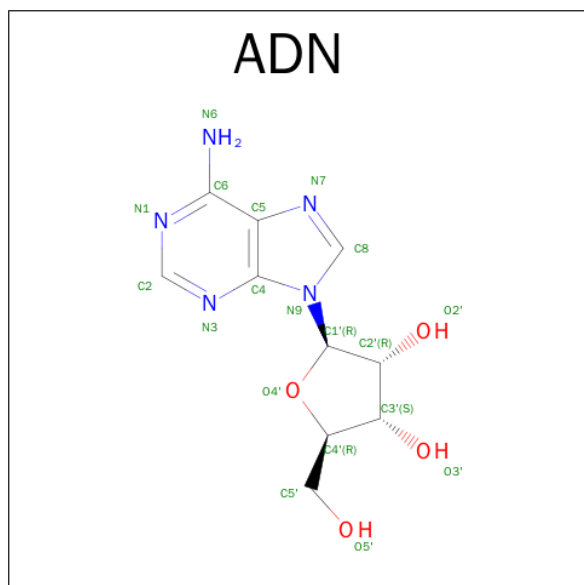
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	363	GLY	-	EXPRESSION TAG	UNP Q8IW19
A	364	PRO	-	EXPRESSION TAG	UNP Q8IW19
A	365	LEU	-	EXPRESSION TAG	UNP Q8IW19
A	366	GLY	-	EXPRESSION TAG	UNP Q8IW19
A	367	SER	-	EXPRESSION TAG	UNP Q8IW19

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

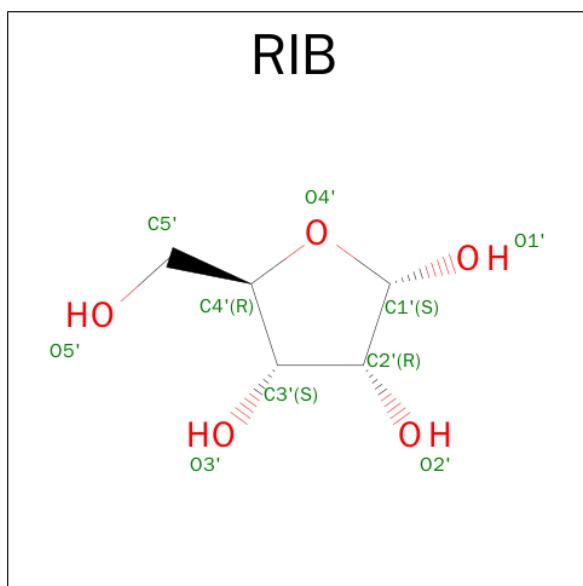
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

- Molecule 3 is ADENOSINE (three-letter code: ADN) (formula: $C_{10}H_{13}N_5O_4$).



Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
3	A	1	31	10	12	5	4

- Molecule 4 is SUGAR (RIBOSE) (three-letter code: RIB) (formula: $C_5H_{10}O_5$).



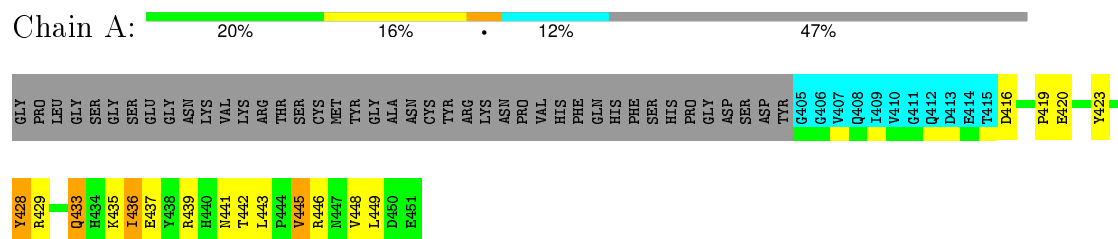
Mol	Chain	Residues	Atoms			
			Total	C	H	O
4	A	1	18	5	9	4

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Aprataxin and PNK-like factor

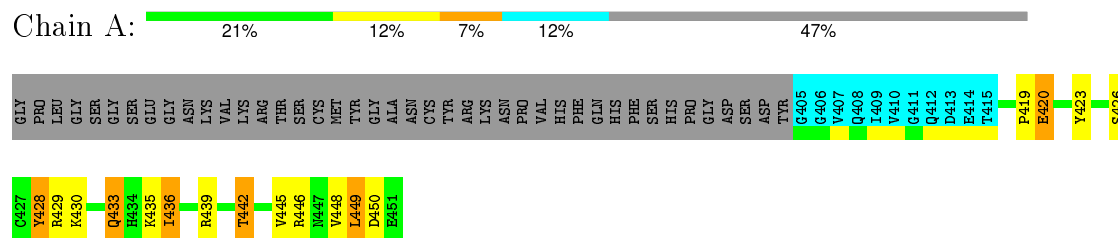


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

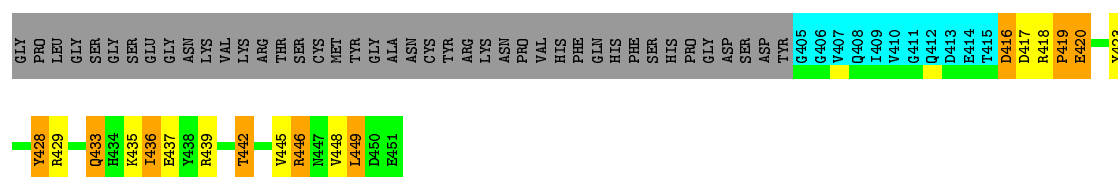
- Molecule 1: Aprataxin and PNK-like factor



4.2.2 Score per residue for model 2

- Molecule 1: Aprataxin and PNK-like factor

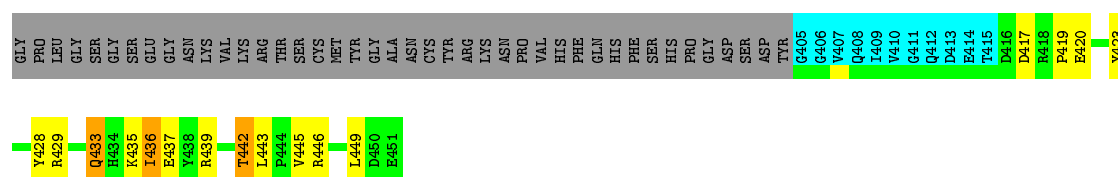




4.2.3 Score per residue for model 3

- Molecule 1: Aprataxin and PNK-like factor

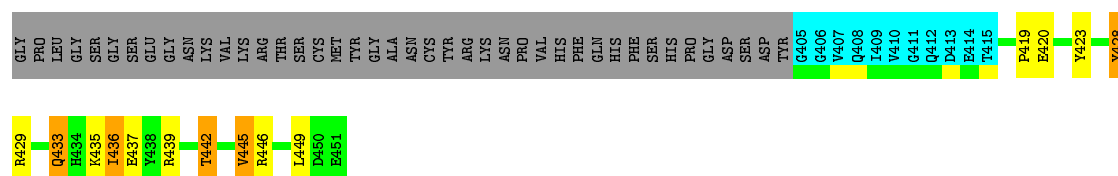
Chain A: 22% 15% • 12% 47%



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Aprataxin and PNK-like factor

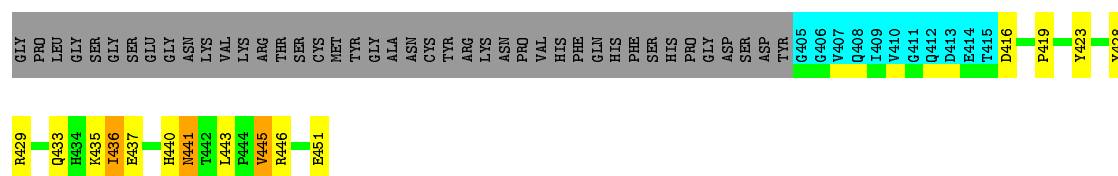
Chain A: 25% 10% 6% 12% 47%



4.2.5 Score per residue for model 5

- Molecule 1: Aprataxin and PNK-like factor

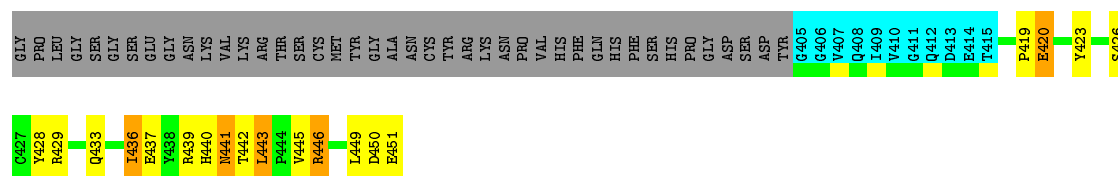
Chain A: 24% 13% • 12% 47%



4.2.6 Score per residue for model 6

- Molecule 1: Aprataxin and PNK-like factor

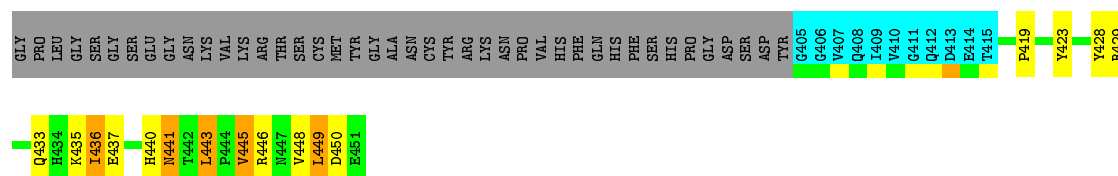
Chain A:  19% 16% 6% 12% 47%



4.2.7 Score per residue for model 7

- Molecule 1: Aprataxin and PNK-like factor

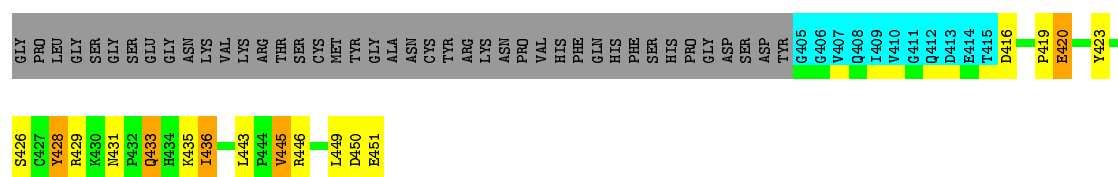
Chain A:  22% 12% 6% 12% 47%



4.2.8 Score per residue for model 8

- Molecule 1: Aprataxin and PNK-like factor

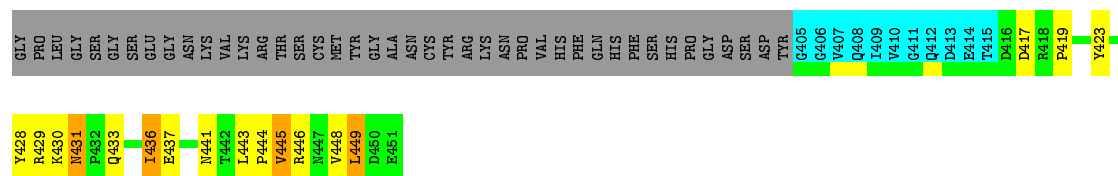
Chain A:  21% 13% 6% 12% 47%



4.2.9 Score per residue for model 9

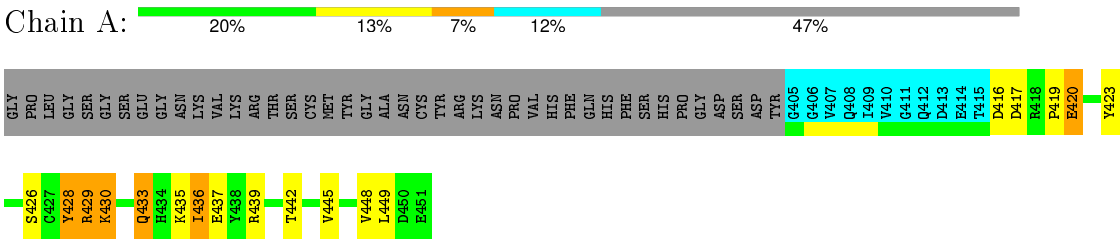
- Molecule 1: Aprataxin and PNK-like factor

Chain A:  21% 15% • 12% 47%



4.2.10 Score per residue for model 10

- Molecule 1: Aprataxin and PNK-like factor



5 Refinement protocol and experimental data overview ⓘ

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

Of the 50 calculated structures, 10 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
XPLOR-NIH	structure solution	
XPLOR-NIH	refinement	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

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 ⓘ

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	305	284	284	11±2
3	A	19	12	12	2±1
4	A	9	9	8	3±1
All	All	3340	3050	3040	109

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:439:ARG:CZ	1:A:442:THR:HG23	0.70	2.16	6	3
1:A:439:ARG:NH2	1:A:442:THR:HG23	0.65	2.07	10	1
1:A:429:ARG:NH1	4:A:1003:RIB:H3'	0.62	2.09	2	7
1:A:429:ARG:CB	4:A:1003:RIB:H5'2	0.62	2.24	8	5
1:A:441:ASN:O	1:A:443:LEU:HD12	0.62	1.95	7	2
1:A:423:TYR:CZ	3:A:1002:ADN:N3	0.62	2.67	4	9
1:A:436:ILE:HD13	1:A:437:GLU:N	0.61	2.09	5	5
1:A:428:TYR:O	3:A:1002:ADN:N1	0.57	2.37	10	1
1:A:429:ARG:HB2	4:A:1003:RIB:H5'2	0.56	1.78	4	6
1:A:449:LEU:O	1:A:449:LEU:HD23	0.56	2.00	8	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:448:VAL:O	1:A:448:VAL:HG12	0.55	2.01	2	3
1:A:429:ARG:HB2	4:A:1003:RIB:H5'1	0.55	1.78	6	3
1:A:448:VAL:HG12	1:A:448:VAL:O	0.55	2.02	1	1
1:A:445:VAL:HG22	1:A:445:VAL:O	0.55	2.02	7	1
1:A:449:LEU:HD23	1:A:449:LEU:O	0.55	2.02	7	1
1:A:429:ARG:HD2	3:A:1002:ADN:N1	0.54	2.18	10	1
1:A:445:VAL:O	1:A:445:VAL:HG12	0.53	2.04	9	5
1:A:423:TYR:CE1	3:A:1002:ADN:N3	0.53	2.77	10	3
1:A:445:VAL:HG12	1:A:445:VAL:O	0.53	2.04	1	4
1:A:448:VAL:O	1:A:448:VAL:HG23	0.49	2.08	7	1
1:A:440:HIS:O	1:A:441:ASN:CB	0.49	2.60	6	2
1:A:429:ARG:CD	3:A:1002:ADN:N1	0.48	2.77	10	1
1:A:433:GLN:HA	1:A:436:ILE:CG2	0.48	2.39	10	6
1:A:436:ILE:HD13	1:A:436:ILE:C	0.47	2.30	8	6
1:A:429:ARG:CB	4:A:1003:RIB:H5'1	0.47	2.39	6	1
1:A:439:ARG:HH21	1:A:442:THR:HG23	0.47	1.68	10	1
1:A:436:ILE:C	1:A:436:ILE:HD13	0.47	2.30	2	4
1:A:439:ARG:CZ	1:A:442:THR:OG1	0.46	2.63	3	1
1:A:439:ARG:NH1	1:A:442:THR:OG1	0.46	2.48	3	2
1:A:441:ASN:OD1	1:A:442:THR:N	0.45	2.49	6	1
1:A:439:ARG:CD	1:A:442:THR:HG23	0.45	2.41	3	1
1:A:428:TYR:CD1	1:A:428:TYR:O	0.45	2.69	8	3
1:A:429:ARG:HB3	4:A:1003:RIB:H5'2	0.44	1.89	8	1
1:A:428:TYR:O	1:A:428:TYR:CD1	0.44	2.71	4	1
1:A:429:ARG:HD2	4:A:1003:RIB:H2'	0.44	1.90	1	3
1:A:440:HIS:O	1:A:441:ASN:CG	0.43	2.56	7	1
1:A:439:ARG:NE	1:A:442:THR:OG1	0.42	2.52	6	1
1:A:440:HIS:O	1:A:441:ASN:ND2	0.41	2.53	6	1
1:A:440:HIS:O	1:A:441:ASN:HB3	0.41	2.15	6	1
1:A:423:TYR:OH	3:A:1002:ADN:H1'	0.41	2.15	8	1
1:A:444:PRO:C	1:A:445:VAL:HG23	0.41	2.36	9	1
1:A:430:LYS:O	1:A:431:ASN:O	0.41	2.38	9	1
1:A:419:PRO:HD2	1:A:437:GLU:O	0.40	2.16	2	1
1:A:430:LYS:CG	1:A:430:LYS:O	0.40	2.69	10	1
1:A:416:ASP:O	1:A:417:ASP:CB	0.40	2.69	2	1

6.3 Torsion angles

6.3.1 Protein backbone

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	35/89 (39%)	24±1 (70±4%)	6±1 (18±3%)	4±1 (12±2%)	1	7
All	All	350/890 (39%)	244 (70%)	64 (18%)	42 (12%)	1	7

All 8 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	419	PRO	10
1	A	446	ARG	9
1	A	420	GLU	7
1	A	445	VAL	5
1	A	449	LEU	4
1	A	441	ASN	4
1	A	450	ASP	2
1	A	431	ASN	1

6.3.2 Protein sidechains

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	35/78 (45%)	27±2 (76±5%)	8±2 (24±5%)	3	28
All	All	350/780 (45%)	267 (76%)	83 (24%)	3	28

All 19 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	428	TYR	10
1	A	433	GLN	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	436	ILE	10
1	A	435	LYS	8
1	A	449	LEU	5
1	A	420	GLU	5
1	A	443	LEU	5
1	A	416	ASP	4
1	A	426	SER	4
1	A	442	THR	4
1	A	417	ASP	3
1	A	451	GLU	3
1	A	437	GLU	3
1	A	450	ASP	2
1	A	446	ARG	2
1	A	430	LYS	2
1	A	418	ARG	1
1	A	431	ASN	1
1	A	429	ARG	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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	ADN	A	1002	4	18,21,21	0.70±0.04	0±0 (0±0%)
4	RIB	A	1003	3	9,9,10	0.54±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	ADN	A	1002	4	16,31,31	0.50±0.18	0±0 (0±0%)
4	RIB	A	1003	3	12,12,14	0.62±0.06	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADN	A	1002	4	-	0±0,2,22,22	0±0,3,3,3
4	RIB	A	1003	3	-	0±0,2,15,18	0±0,1,1,1

There are no bond-length outliers.

There are no bond-angle outliers.

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
4	A	1003	RIB	C1'	1

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided