



Full wwPDB NMR Structure Validation Report i

Apr 20, 2024 – 08:08 PM EDT

PDB ID : 2KWG
Title : Solution structure of a fully modified 2'-F/2'-OMe siRNA construct
Authors : Podbevsek, P.; Bhat, B.; Plavec, J.
Deposited on : 2010-04-09

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](#) ①) were used in the production of this report:

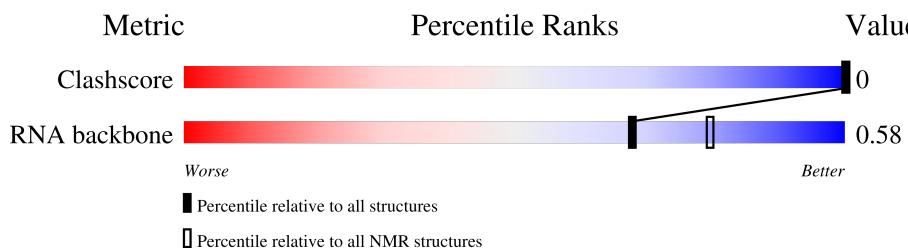
MolProbitY : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLUTION NMR

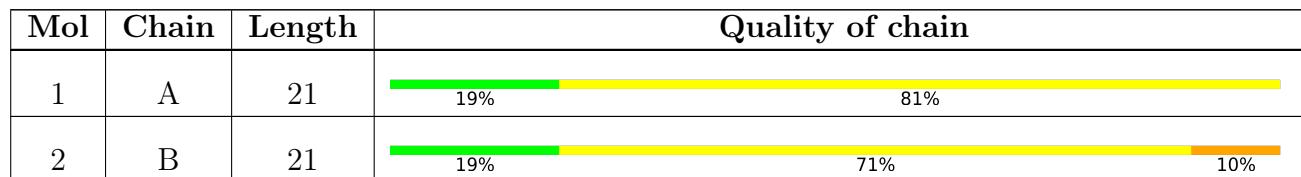
The overall completeness of chemical shifts assignment was not calculated.

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
RNA backbone	4643	676

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%



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
2	B	A2M	22	8	-
2	B	UFT	23	2	-

2 Ensemble composition and analysis

This entry contains 10 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1373 atoms, of which 470 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called 5'-R(*(GF2)P*(OMG)P*(GF2)P*(OMU)P*(AF2)P*(A2M)P*(AF2)P*(OMU)P*(AF2)P*(OMC)P*(AF2)P*(OMU)P*(UFT)P*(OMC)P*(UFT)P*(OMU)P*(CFZ)P*(A2M)P*(UFT)P*(OMU)P*(UFT))-3'.

Mol	Chain	Residues	Atoms							Trace
			Total	C	F	H	N	O	P	
1	A	21	681	208	11	233	72	137	20	0

- Molecule 2 is a RNA chain called 5'-R(P*(A2M)P*(UFT)P*(OMG)P*(AF2)P*(A2M)P*(GF2)P*(A2M)P*(AF2)P*(OMU)P*(GF2)P*(OMU)P*(AF2)P*(OMU)P*(UFT)P*(OMU)P*(AF2)P*(OMC)P*(CFZ)P*(OMC)P*(UFT)P*(OMU))-3'.

Mol	Chain	Residues	Atoms							Trace
			Total	C	F	H	N	O	P	
2	B	21	692	210	10	237	75	139	21	0

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: 5'-R(*(GF2)P*(OMG)P*(GF2)P*(OMU)P*(AF2)P*(A2M)P*(AF2)P*(OMU)P*(AF2)P*(OMC)P*(AF2)P*(OMU)P*(UFT)P*(OMC)P*(UFT)P*(OMU)P*(CFZ)P*(A2M)P*(UFT)P*(OMU)P*(UFT))-3'



- Molecule 2: 5'-R(P*(A2M)P*(UFT)P*(OMG)P*(AF2)P*(A2M)P*(GF2)P*(A2M)P*(AF2)P*(OMU)P*(GF2)P*(OMU)P*(AF2)P*(OMU)P*(UFT)P*(OMU)P*(AF2)P*(OMC)P*(CFZ)P*(OMC)P*(UFT)P*(OMU))-3'



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: 5'-R(*(GF2)P*(OMG)P*(GF2)P*(OMU)P*(AF2)P*(A2M)P*(AF2)P*(OMU)P*(AF2)P*(OMC)P*(AF2)P*(OMU)P*(UFT)P*(OMC)P*(UFT)P*(OMU)P*(CFZ)P*(A2M)P*(UFT)P*(OMU)P*(UFT))-3'



- Molecule 2: 5'-R(P*(A2M)P*(UFT)P*(OMG)P*(AF2)P*(A2M)P*(GF2)P*(A2M)P*(AF2)P*(OMU)P*(GF2)P*(OMU)P*(AF2)P*(OMU)P*(UFT)P*(OMU)P*(AF2)P*(OMC)P*(CFZ)P*(OMC)P*(UFT)P*(OMU))-3'



4.2.2 Score per residue for model 2

- Molecule 1: 5'-R(*(GF2)P*(OMG)P*(GF2)P*(OMU)P*(AF2)P*(A2M)P*(AF2)P*(OMU)P*(AF2)P*(OMC)P*(AF2)P*(OMU)P*(UFT)P*(OMC)P*(UFT)P*(OMU)P*(CFZ)P*(A2M)P*(UFT)P*(OMU)P*(UFT))-3'



- Molecule 2: 5'-R(P*(A2M)P*(UFT)P*(OMG)P*(AF2)P*(A2M)P*(GF2)P*(A2M)P*(AF2)P*(OMU)P*(GF2)P*(OMU)P*(AF2)P*(OMU)P*(UFT)P*(OMU)P*(AF2)P*(OMC)P*(CFZ)P*(OMC)P*(UFT)P*(OMU))-3'



4.2.3 Score per residue for model 3

- Molecule 1: 5'-R(*(GF2)P*(OMG)P*(GF2)P*(OMU)P*(AF2)P*(A2M)P*(AF2)P*(OMU)P*(AF2)P*(OMC)P*(AF2)P*(OMU)P*(UFT)P*(OMC)P*(UFT)P*(OMU)P*(CFZ)P*(A2M)P*(UFT)P*(OMU)P*(UFT))-3'



- Molecule 2: 5'-R(P*(A2M)P*(UFT)P*(OMG)P*(AF2)P*(A2M)P*(GF2)P*(A2M)P*(AF2)P*(OMU)P*(GF2)P*(OMU)P*(AF2)P*(OMU)P*(UFT)P*(OMU)P*(AF2)P*(OMC)P*(CFZ)P*(OMC)P*(UFT)P*(OMU))-3'

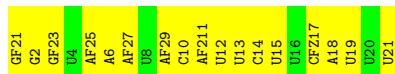




4.2.4 Score per residue for model 4

- Molecule 1: 5'-R(*(GF2)P*(OMG)P*(GF2)P*(OMU)P*(AF2)P*(A2M)P*(AF2)P*(OMU)P*(AF2)P*(OMC)P*(AF2)P*(OMU)P*(UFT)P*(OMC)P*(UFT)P*(OMU)P*(CFZ)P*(A2M)P*(UFT)P*(OMU)P*(UFT))-3'

Chain A: 19% 81%



- Molecule 2: 5'-R(P*(A2M)P*(UFT)P*(OMG)P*(AF2)P*(A2M)P*(GF2)P*(A2M)P*(AF2)P*(OMU)P*(GF2)P*(OMU)P*(AF2)P*(OMU)P*(UFT)P*(OMU)P*(AF2)P*(OMC)P*(CFZ)P*(OMC)P*(UFT)P*(OMU))-3'

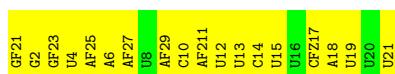
Chain B: 24% 71% 5%



4.2.5 Score per residue for model 5

- Molecule 1: 5'-R(*(GF2)P*(OMG)P*(GF2)P*(OMU)P*(AF2)P*(A2M)P*(AF2)P*(OMU)P*(AF2)P*(OMC)P*(AF2)P*(OMU)P*(UFT)P*(OMC)P*(UFT)P*(OMU)P*(CFZ)P*(A2M)P*(UFT)P*(OMU)P*(UFT))-3'

Chain A: 14% 86%



- Molecule 2: 5'-R(P*(A2M)P*(UFT)P*(OMG)P*(AF2)P*(A2M)P*(GF2)P*(A2M)P*(AF2)P*(OMU)P*(GF2)P*(OMU)P*(AF2)P*(OMU)P*(UFT)P*(OMU)P*(AF2)P*(OMC)P*(CFZ)P*(OMC)P*(UFT)P*(OMU))-3'

Chain B: 19% 71% 10%



4.2.6 Score per residue for model 6

- Molecule 1: 5'-R(*(GF2)P*(OMG)P*(GF2)P*(OMU)P*(AF2)P*(A2M)P*(AF2)P*(OMU)P*(AF2)P*(OMC)P*(AF2)P*(OMU)P*(UFT)P*(OMC)P*(UFT)P*(OMU)P*(CFZ)P*(A2M)P*(UFT)P*(OMU)P*(UFT))-3'

Chain A:  24% 76%



- Molecule 2: 5'-R(P*(A2M)P*(UFT)P*(OMG)P*(AF2)P*(A2M)P*(GF2)P*(A2M)P*(AF2)P*(OMU)P*(GF2)P*(OMU)P*(AF2)P*(OMU)P*(UFT)P*(OMU)P*(AF2)P*(OMC)P*(CFZ)P*(OMC)P*(UFT)P*(OMU))-3'

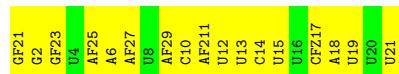
Chain B:  19% 76% 5%



4.2.7 Score per residue for model 7

- Molecule 1: 5'-R(*(GF2)P*(OMG)P*(GF2)P*(OMU)P*(AF2)P*(A2M)P*(AF2)P*(OMU)P*(AF2)P*(OMC)P*(AF2)P*(OMU)P*(UFT)P*(OMC)P*(UFT)P*(OMU)P*(CFZ)P*(A2M)P*(UFT)P*(OMU)P*(UFT))-3'

Chain A:  19% 81%



- Molecule 2: 5'-R(P*(A2M)P*(UFT)P*(OMG)P*(AF2)P*(A2M)P*(GF2)P*(A2M)P*(AF2)P*(OMU)P*(GF2)P*(OMU)P*(AF2)P*(OMU)P*(UFT)P*(OMU)P*(AF2)P*(OMC)P*(CFZ)P*(OMC)P*(UFT)P*(OMU))-3'

Chain B:  19% 81%



4.2.8 Score per residue for model 8

- Molecule 1: 5'-R(*(GF2)P*(OMG)P*(GF2)P*(OMU)P*(AF2)P*(A2M)P*(AF2)P*(OMU)P*(AF2)P*(OMC)P*(AF2)P*(OMU)P*(UFT)P*(OMC)P*(UFT)P*(OMU)P*(CFZ)P*(A2M)P*(UFT)P*(OMU)P*(UFT))-3'



GF21	G2	GF23
	G2	
U4	AF25	A6
	AF25	AF27
U8	UB	AF29
		AF29
C10		AF211
		U12
A26		U13
AF225		U13
A28		U34
AF229		U35
U30		U36
GF231		AF237
		C38
U32		CFZ17
AF233		A18
U34		U19
U35		U40
U36		U41
U16		U42
AF237		
C38		
CFZ17		
A18		
U19		
U20		
U21		

- Molecule 2: 5'-R(P*(A2M)P*(UFT)P*(OMG)P*(AF2)P*(A2M)P*(GF2)P*(A2M)P*(AF2)P*(OMU)P*(GF2)P*(OMU)P*(AF2)P*(OMU)P*(UFT)P*(OMU)P*(AF2)P*(OMC)P*(CFZ)P*(OMC)P*(UFT)P*(OMU))-3'



A22	U23	G24
	U23	
AF225		AF227
A26		A28
AF229		AF229
U30		U30
GF231		GF231
U32		U32
AF233		AF233
U34		U34
U35		U35
U36		U36
AF237		AF237
C38		C38
CFZ17		CFZ17
A18		A18
U19		U19
U40		U40
U41		U41
U42		U42

4.2.9 Score per residue for model 9

- Molecule 1: 5'-R(*(GF2)P*(OMG)P*(GF2)P*(OMU)P*(AF2)P*(A2M)P*(AF2)P*(OMU)P*(AF2)P*(OMC)P*(AF2)P*(OMU)P*(UFT)P*(OMC)P*(UFT)P*(OMU)P*(CFZ)P*(A2M)P*(UFT)P*(OMU)P*(UFT))-3'



GF21	G2	GF23
	G2	
U4	AF25	A6
	AF25	AF27
U8	UB	AF29
		AF29
C10		AF211
		U12
A26		U13
AF225		U13
A28		U34
AF229		U35
U30		U36
GF231		AF237
		C38
U32		CFZ17
AF233		A18
U34		U19
U35		U40
U36		U41
U16		U42
AF237		
C38		
CFZ17		
A18		
U19		
U20		
U21		

- Molecule 2: 5'-R(P*(A2M)P*(UFT)P*(OMG)P*(AF2)P*(A2M)P*(GF2)P*(A2M)P*(AF2)P*(OMU)P*(AF2)P*(OMU)P*(AF2)P*(OMU)P*(UFT)P*(OMU)P*(AF2)P*(OMC)P*(CFZ)P*(OMC)P*(UFT)P*(OMU))-3'



A22	U23	G24
	U23	
AF225		AF227
A26		A28
AF229		AF229
U30		U30
GF231		GF231
U32		U32
AF233		AF233
U34		U34
U35		U35
U36		U36
AF237		AF237
C38		C38
CFZ17		CFZ17
A18		A18
U19		U19
U40		U40
U41		U41
U42		U42

4.2.10 Score per residue for model 10

- Molecule 1: 5'-R(*(GF2)P*(OMG)P*(GF2)P*(OMU)P*(AF2)P*(A2M)P*(AF2)P*(OMU)P*(AF2)P*(OMC)P*(AF2)P*(OMU)P*(UFT)P*(OMC)P*(UFT)P*(OMU)P*(CFZ)P*(A2M)P*(UFT)P*(OMU)P*(UFT))-3'



GF21	G2	GF23
	G2	
U4	AF25	A6
	AF25	AF27
U8	UB	AF29
		AF29
C10		AF211
		U12
A26		U13
AF225		U13
A28		U34
AF229		U35
U30		U36
GF231		AF237
		C38
U32		CFZ17
AF233		A18
U34		U19
U35		U40
U36		U41
U16		U42
AF237		
C38		
CFZ17		
A18		
U19		
U20		
U21		

- Molecule 2: 5'-R(P*(A2M)P*(UFT)P*(OMG)P*(AF2)P*(A2M)P*(GF2)P*(A2M)P*(AF2)P*(OMU)P*(GF2)P*(OMU)P*(AF2)P*(OMU)P*(UFT)P*(OMU)P*(AF2)P*(OMC)P*(CFZ)P*(OMC)P*(UFT)P*(OMU))-3'

Chain B: 14% 76% 10%



5 Refinement protocol and experimental data overview i

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

Of the 100 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
Amber	structure solution	9
Amber	refinement	9

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: A2M, CFZ, GF2, UFT, AF2, OMC, OMG, OMU

There are no covalent bond-length or bond-angle outliers.

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
2	B	1.6±0.8	0.0±0.0
All	All	16	0

There are no bond-length outliers.

There are no bond-angle outliers.

All unique chiral outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	22	A2M	C3',C4'	8
2	B	23	UFT	C4'	2

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
All	All	9030	4700	4680	-

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 -.

There are no clashes.

6.3 Torsion angles [\(i\)](#)

6.3.1 Protein backbone [\(i\)](#)

There are no protein molecules in this entry.

6.3.2 Protein sidechains [\(i\)](#)

There are no protein molecules in this entry.

6.3.3 RNA [\(i\)](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	9/21 (43%)	0±0 (0±0%)	0±0 (0±0%)	0.61±0.04
2	B	10/21 (48%)	1±1 (9±5%)	0±0 (0±0%)	0.56±0.04
All	All	190/420 (45%)	9 (5%)	0 (0%)	0.58

The overall RNA backbone suiteness is 0.58.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	24	OMG	8
2	B	42	OMU	1

There are no RNA pucker outliers to report.

6.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

42 non-standard protein/DNA/RNA residues are modelled in this entry.

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
2	GF2	B	27	2	18,25,26	0.98±0.01	1±0 (5±0%)
2	UFT	B	41	2	18,21,22	0.70±0.04	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	OMU	A	12	1	19,22,23	0.63±0.01	0±0 (0±0%)
1	A2M	A	18	2,1	18,25,26	0.81±0.01	0±0 (0±0%)
1	UFT	A	15	2,1	18,21,22	0.66±0.01	0±0 (0±0%)
2	UFT	B	35	2,1	18,21,22	0.66±0.01	0±0 (0±0%)
1	A2M	A	6	2,1	18,25,26	0.80±0.01	0±0 (0±0%)
1	CFZ	A	17	1	18,21,22	0.68±0.01	0±0 (0±0%)
2	AF2	B	25	2	18,24,25	0.84±0.01	0±0 (0±0%)
1	UFT	A	13	2,1	18,21,22	0.65±0.01	0±0 (0±0%)
2	OMU	B	34	2	19,22,23	0.64±0.01	0±0 (0±0%)
2	OMG	B	24	2	18,26,27	0.98±0.01	1±0 (5±0%)
1	AF2	A	5	1	18,24,25	0.82±0.01	0±0 (0±0%)
1	GF2	A	1	-	18,22,26	0.99±0.01	1±0 (5±0%)
1	UFT	A	21	1	18,21,22	0.68±0.01	0±0 (0±0%)
1	GF2	A	3	1	18,25,26	0.98±0.01	1±0 (5±0%)
1	AF2	A	11	1	18,24,25	0.83±0.01	0±0 (0±0%)
2	GF2	B	31	2	18,25,26	0.99±0.01	1±0 (5±0%)
2	AF2	B	29	2	18,24,25	0.82±0.01	0±0 (0±0%)
2	A2M	B	26	2,1	18,25,26	0.81±0.01	0±0 (0±0%)
1	OMU	A	4	1	19,22,23	0.64±0.01	0±0 (0±0%)
2	OMC	B	40	2	19,22,23	0.62±0.03	0±0 (0±0%)
1	AF2	A	7	1	18,24,25	0.82±0.01	0±0 (0±0%)
1	OMC	A	10	1	19,22,23	0.64±0.00	0±0 (0±0%)
2	A2M	B	22	2,1	22,26,26	0.78±0.02	0±0 (0±0%)
2	OMU	B	36	2	19,22,23	0.64±0.01	0±0 (0±0%)
2	AF2	B	33	2	18,24,25	0.83±0.01	0±0 (0±0%)
2	OMU	B	32	2	19,22,23	0.64±0.01	0±0 (0±0%)
1	OMG	A	2	1	18,26,27	0.97±0.01	1±0 (5±0%)
1	OMU	A	20	1	19,22,23	0.63±0.01	0±0 (0±0%)
2	OMC	B	38	2	19,22,23	0.65±0.01	0±0 (0±0%)
1	OMU	A	8	1	19,22,23	0.64±0.01	0±0 (0±0%)
1	OMU	A	16	1	19,22,23	0.63±0.01	0±0 (0±0%)
2	CFZ	B	39	2	18,21,22	0.67±0.01	0±0 (0±0%)
2	AF2	B	37	2	18,24,25	0.83±0.01	0±0 (0±0%)
2	UFT	B	23	2,1	18,21,22	0.71±0.03	0±0 (0±0%)
1	AF2	A	9	1	18,24,25	0.82±0.01	0±0 (0±0%)
2	OMU	B	30	2	19,22,23	0.64±0.01	0±0 (0±0%)
1	OMC	A	14	1	19,22,23	0.65±0.00	0±0 (0±0%)
1	UFT	A	19	2,1	18,21,22	0.64±0.01	0±0 (0±0%)
2	A2M	B	28	2,1	18,25,26	0.81±0.01	0±0 (0±0%)
2	OMU	B	42	2	19,22,23	0.64±0.03	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
2	GF2	B	27	2	19,37,40	1.35±0.02	3±0 (15±0%)
2	UFT	B	41	2	26,30,33	0.97±0.06	1±1 (4±2%)
1	OMU	A	12	1	26,31,34	0.93±0.04	1±0 (3±1%)
1	A2M	A	18	2,1	18,36,39	1.22±0.04	2±0 (11±0%)
1	UFT	A	15	2,1	26,30,33	1.10±0.10	1±1 (5±2%)
2	UFT	B	35	2,1	26,30,33	1.13±0.07	2±0 (8±1%)
1	A2M	A	6	2,1	18,36,39	1.20±0.03	2±0 (11±0%)
1	CFZ	A	17	1	26,30,33	1.24±0.02	2±0 (7±0%)
2	AF2	B	25	2	18,35,38	1.35±0.06	3±0 (15±2%)
1	UFT	A	13	2,1	26,30,33	1.04±0.02	1±0 (4±1%)
2	OMU	B	34	2	26,31,34	0.95±0.01	0±0 (0±1%)
2	OMG	B	24	2	19,38,41	1.16±0.02	2±0 (10±0%)
1	AF2	A	5	1	18,35,38	1.39±0.05	3±0 (16±1%)
1	GF2	A	1	-	19,33,40	1.25±0.04	3±0 (15±1%)
1	UFT	A	21	1	26,30,33	1.05±0.05	1±0 (3±0%)
1	GF2	A	3	1	19,37,40	1.38±0.04	3±1 (17±3%)
1	AF2	A	11	1	18,35,38	1.37±0.02	3±0 (16±0%)
2	GF2	B	31	2	19,37,40	1.32±0.05	3±0 (15±1%)
2	AF2	B	29	2	18,35,38	1.43±0.02	3±0 (16±0%)
2	A2M	B	26	2,1	18,36,39	1.21±0.03	2±0 (11±0%)
1	OMU	A	4	1	26,31,34	1.01±0.05	1±1 (2±3%)
2	OMC	B	40	2	26,31,34	1.16±0.10	2±0 (6±1%)
1	AF2	A	7	1	18,35,38	1.38±0.06	3±0 (16±0%)
1	OMC	A	10	1	26,31,34	1.16±0.03	1±0 (4±1%)
2	A2M	B	22	2,1	25,39,39	1.27±0.02	3±0 (12±1%)
2	OMU	B	36	2	26,31,34	0.96±0.02	0±0 (0±0%)
2	AF2	B	33	2	18,35,38	1.35±0.06	3±0 (16±1%)
2	OMU	B	32	2	26,31,34	1.01±0.06	0±0 (1±1%)
1	OMG	A	2	1	19,38,41	1.18±0.02	2±0 (10±0%)
1	OMU	A	20	1	26,31,34	0.91±0.04	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	OMC	B	38	2	26,31,34	1.12±0.02	1±0 (3±0%)
1	OMU	A	8	1	26,31,34	0.97±0.04	0±0 (0±0%)
1	OMU	A	16	1	26,31,34	0.96±0.04	0±0 (1±1%)
2	CFZ	B	39	2	26,30,33	1.41±0.06	3±1 (11±4%)
2	AF2	B	37	2	18,35,38	1.37±0.05	3±0 (16±1%)
2	UFT	B	23	2,1	26,30,33	1.06±0.07	1±1 (4±2%)
1	AF2	A	9	1	18,35,38	1.36±0.03	3±0 (16±0%)
2	OMU	B	30	2	26,31,34	0.99±0.06	1±0 (2±1%)
1	OMC	A	14	1	26,31,34	1.14±0.03	1±0 (3±0%)
1	UFT	A	19	2,1	26,30,33	1.13±0.03	2±0 (7±1%)
2	A2M	B	28	2,1	18,36,39	1.21±0.02	2±0 (11±0%)
2	OMU	B	42	2	26,31,34	1.02±0.06	0±0 (1±1%)

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
1	AF2	A	7	1	-	0±0,3,25,26	0±0,3,3,3
1	OMC	A	10	1	-	0±0,9,27,28	0±0,2,2,2
1	A2M	A	18	2,1	-	0±0,5,27,28	0±0,3,3,3
1	GF2	A	3	1	-	0±0,3,25,26	0±0,3,3,3
1	UFT	A	21	1	-	0±0,7,25,26	0±0,2,2,2
2	GF2	B	27	2	-	0±0,3,25,26	0±0,3,3,3
1	OMU	A	8	1	-	0±0,9,27,28	0±0,2,2,2
1	OMU	A	16	1	-	0±0,9,27,28	0±0,2,2,2
2	UFT	B	23	2,1	-	0±0,7,25,26	0±0,2,2,2
1	A2M	A	6	2,1	-	0±0,5,27,28	0±0,3,3,3
2	OMU	B	30	2	-	0±0,9,27,28	0±0,2,2,2
2	AF2	B	33	2	-	0±0,3,25,26	0±0,3,3,3
1	GF2	A	1	-	-	0±0,2,22,26	0±0,3,3,3
2	UFT	B	35	2,1	-	0±0,7,25,26	0±0,2,2,2
1	OMU	A	4	1	-	0±0,9,27,28	0±0,2,2,2
2	CFZ	B	39	2	-	0±0,7,25,26	0±0,2,2,2
2	A2M	B	28	2,1	-	0±0,5,27,28	0±0,3,3,3
2	OMU	B	42	2	-	0±0,9,27,28	0±0,2,2,2
2	OMU	B	32	2	-	0±0,9,27,28	0±0,2,2,2
2	OMC	B	40	2	-	0±0,9,27,28	0±0,2,2,2
1	OMG	A	2	1	-	0±0,5,27,28	0±0,3,3,3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GF2	B	31	2	-	0±0,3,25,26	0±0,3,3,3
1	OMC	A	14	1	-	0±0,9,27,28	0±0,2,2,2
1	CFZ	A	17	1	-	0±0,7,25,26	0±0,2,2,2
2	UFT	B	41	2	-	0±0,7,25,26	0±0,2,2,2
2	OMU	B	36	2	-	0±0,9,27,28	0±0,2,2,2
2	AF2	B	29	2	-	0±0,3,25,26	0±0,3,3,3
1	OMU	A	12	1	-	0±0,9,27,28	0±0,2,2,2
2	A2M	B	22	2,1	2±0,2,5,5	0±0,8,28,28	0±0,3,3,3
1	AF2	A	11	1	-	0±0,3,25,26	0±0,3,3,3
1	UFT	A	13	2,1	-	0±0,7,25,26	0±0,2,2,2
1	AF2	A	5	1	-	0±0,3,25,26	0±0,3,3,3
1	AF2	A	9	1	-	0±0,3,25,26	0±0,3,3,3
2	AF2	B	25	2	-	0±0,3,25,26	0±0,3,3,3
2	OMC	B	38	2	-	0±0,9,27,28	0±0,2,2,2
2	OMG	B	24	2	-	0±0,5,27,28	0±0,3,3,3
2	OMU	B	34	2	-	0±0,9,27,28	0±0,2,2,2
1	UFT	A	19	2,1	-	0±0,7,25,26	0±0,2,2,2
2	AF2	B	37	2	-	0±0,3,25,26	0±0,3,3,3
1	OMU	A	20	1	-	0±0,9,27,28	0±0,2,2,2
1	UFT	A	15	2,1	-	0±0,7,25,26	0±0,2,2,2
2	A2M	B	26	2,1	-	0±0,5,27,28	0±0,3,3,3

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	1	GF2	C8-N7	2.36	1.31	1.35	10	10
2	B	24	OMG	C8-N7	2.31	1.31	1.35	1	10
1	A	2	OMG	C8-N7	2.27	1.31	1.35	5	10
2	B	31	GF2	C8-N7	2.27	1.31	1.35	3	10
1	A	3	GF2	C8-N7	2.22	1.31	1.35	6	10
2	B	27	GF2	C8-N7	2.19	1.31	1.35	10	10

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(°)	Ideal(°)	Models	
								Worst	Total
2	B	23	UFT	O4'-C1'-C2'	3.85	101.82	105.79	2	2
1	A	5	AF2	C5-C6-N6	3.62	125.85	120.35	8	10
1	A	7	AF2	F-C2'-C3'	3.62	116.80	109.22	2	1
2	B	22	A2M	C5-C6-N6	3.60	125.82	120.35	10	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	29	AF2	C5-C6-N6	3.47	125.62	120.35	4	10
1	A	18	A2M	C5-C6-N6	3.47	125.62	120.35	10	10
2	B	40	OMC	O2-C2-N3	3.46	116.71	122.33	4	10
2	B	42	OMU	O2'-C2'-C1'	3.44	115.78	109.08	7	4
2	B	38	OMC	O2-C2-N3	3.42	116.78	122.33	4	10
1	A	15	UFT	F2'-C2'-C3'	3.40	116.34	109.22	4	2
1	A	11	AF2	C5-C6-N6	3.40	125.52	120.35	7	10
2	B	39	CFZ	O2-C2-N3	3.39	116.81	122.33	8	10
1	A	7	AF2	C5-C6-N6	3.39	125.50	120.35	4	10
2	B	39	CFZ	F2'-C2'-C3'	3.38	116.30	109.22	5	9
2	B	33	AF2	C2'-C3'-C4'	3.38	98.04	102.40	8	9
2	B	37	AF2	C5-C6-N6	3.37	125.47	120.35	7	10
1	A	6	A2M	C5-C6-N6	3.31	125.38	120.35	2	10
1	A	9	AF2	C5-C6-N6	3.31	125.38	120.35	6	10
1	A	10	OMC	O2-C2-N3	3.29	116.97	122.33	3	10
1	A	14	OMC	O2-C2-N3	3.29	116.97	122.33	9	10
2	B	40	OMC	O2'-C2'-C1'	3.27	115.46	109.08	6	6
1	A	17	CFZ	O2-C2-N3	3.25	117.04	122.33	8	10
1	A	9	AF2	C2'-C3'-C4'	3.24	98.22	102.40	2	10
2	B	29	AF2	C2'-C3'-C4'	3.21	98.25	102.40	7	10
1	A	17	CFZ	C2'-C3'-C4'	3.20	98.27	102.40	10	10
2	B	25	AF2	C5-C6-N6	3.18	125.18	120.35	4	10
2	B	26	A2M	C5-C6-N6	3.18	125.18	120.35	8	10
2	B	35	UFT	F2'-C2'-C3'	3.17	115.87	109.22	8	1
2	B	25	AF2	C2'-C3'-C4'	3.17	98.31	102.40	5	8
2	B	28	A2M	C5-C6-N6	3.16	125.16	120.35	4	10
2	B	33	AF2	C5-C6-N6	3.16	125.15	120.35	2	10
2	B	35	UFT	C2'-C3'-C4'	3.15	98.34	102.40	4	9
1	A	3	GF2	O6-C6-N1	3.11	116.97	120.65	7	10
1	A	2	OMG	O6-C6-N1	3.10	116.98	120.65	6	10
1	A	19	UFT	C2'-C3'-C4'	3.08	98.42	102.40	2	10
2	B	31	GF2	O6-C6-N1	3.08	117.01	120.65	9	10
1	A	5	AF2	C2'-C3'-C4'	3.08	98.43	102.40	5	9
2	B	27	GF2	C2'-C3'-C4'	3.08	98.43	102.40	4	10
2	B	31	GF2	C2'-C3'-C4'	3.07	98.44	102.40	6	9
2	B	27	GF2	O6-C6-N1	3.07	117.03	120.65	6	10
2	B	24	OMG	O6-C6-N1	2.99	117.12	120.65	2	10
2	B	37	AF2	C2'-C3'-C4'	2.99	98.54	102.40	2	9
1	A	15	UFT	C2'-C3'-C4'	2.94	98.60	102.40	5	10
1	A	3	GF2	C2'-C3'-C4'	2.92	98.62	102.40	1	8
1	A	13	UFT	C2'-C3'-C4'	2.90	98.65	102.40	10	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	1	GF2	O6-C6-N1	2.89	117.24	120.65	9	10
1	A	7	AF2	C2'-C3'-C4'	2.80	98.79	102.40	6	9
1	A	11	AF2	C2'-C3'-C4'	2.73	98.87	102.40	3	10
1	A	3	GF2	O6-C6-C5	2.71	129.67	124.37	1	10
2	B	39	CFZ	C2'-C3'-C4'	2.71	98.90	102.40	7	5
1	A	19	UFT	C2'-C1'-N1	2.69	110.09	114.20	2	9
2	B	23	UFT	C2'-C3'-C4'	2.69	98.93	102.40	8	6
1	A	1	GF2	C2'-C3'-C4'	2.68	98.94	102.40	8	9
2	B	35	UFT	C2'-C1'-N1	2.66	110.14	114.20	4	10
2	B	22	A2M	N6-C6-N1	2.64	113.08	118.57	10	10
1	A	2	OMG	O6-C6-C5	2.64	129.53	124.37	6	10
2	B	27	GF2	O6-C6-C5	2.63	129.51	124.37	6	10
2	B	31	GF2	O6-C6-C5	2.61	129.48	124.37	9	10
2	B	39	CFZ	C3'-C2'-C1'	2.61	99.97	103.13	10	4
2	B	41	UFT	F2'-C2'-C3'	2.61	114.68	109.22	1	5
1	A	5	AF2	N6-C6-N1	2.60	113.18	118.57	8	10
2	B	29	AF2	N6-C6-N1	2.59	113.19	118.57	4	10
2	B	24	OMG	O6-C6-C5	2.57	129.39	124.37	5	10
1	A	18	A2M	N6-C6-N1	2.56	113.27	118.57	10	10
1	A	21	UFT	F2'-C2'-C3'	2.56	114.57	109.22	10	10
1	A	1	GF2	O6-C6-C5	2.54	129.34	124.37	9	10
1	A	6	A2M	N6-C6-N1	2.53	113.33	118.57	2	10
2	B	37	AF2	N6-C6-N1	2.51	113.37	118.57	7	10
2	B	41	UFT	C2'-C3'-C4'	2.48	99.19	102.40	7	4
1	A	11	AF2	N6-C6-N1	2.48	113.43	118.57	6	10
1	A	7	AF2	N6-C6-N1	2.47	113.45	118.57	4	10
2	B	35	UFT	O4'-C1'-N1	2.44	113.94	108.36	8	1
1	A	9	AF2	N6-C6-N1	2.40	113.59	118.57	6	10
1	A	3	GF2	F-C2'-C3'	2.40	114.24	109.22	6	5
2	B	26	A2M	N6-C6-N1	2.39	113.62	118.57	8	10
2	B	28	A2M	N6-C6-N1	2.39	113.62	118.57	4	10
2	B	33	AF2	N6-C6-N1	2.38	113.63	118.57	2	10
2	B	41	UFT	O4'-C1'-N1	2.38	113.81	108.36	4	1
2	B	25	AF2	N6-C6-N1	2.36	113.67	118.57	4	10
2	B	23	UFT	O4'-C1'-N1	2.34	113.71	108.36	5	1
2	B	22	A2M	OP2-P-OP1	2.27	119.58	110.68	6	10
2	B	39	CFZ	O4'-C1'-N1	2.22	113.43	108.36	10	2
1	A	15	UFT	F2'-C2'-C1'	2.21	113.68	109.08	1	1
2	B	23	UFT	C2'-C1'-N1	2.18	110.87	114.20	10	2
1	A	4	OMU	C2'-C1'-N1	2.15	110.04	114.22	3	5
1	A	13	UFT	C2'-C1'-N1	2.14	110.93	114.20	10	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	41	UFT	C4'-O4'-C1'	2.13	104.77	109.47	4	1
2	B	30	OMU	O4'-C1'-N1	2.11	113.18	108.36	5	7
1	A	12	OMU	O4'-C1'-N1	2.10	113.17	108.36	9	8
2	B	32	OMU	O4'-C1'-N1	2.10	113.16	108.36	8	3
2	B	22	A2M	OP3-P-O5'	2.09	101.17	106.73	2	1
1	A	15	UFT	C2'-C1'-N1	2.07	111.04	114.20	10	1
2	B	34	OMU	O4'-C1'-N1	2.06	113.07	108.36	8	1
1	A	10	OMC	O4'-C1'-N1	2.05	113.04	108.36	2	1
2	B	41	UFT	C3'-C2'-C1'	2.02	105.57	103.13	5	1
1	A	4	OMU	O4'-C1'-N1	2.01	112.96	108.36	3	2
1	A	16	OMU	O4'-C1'-N1	2.00	112.95	108.36	10	3

All unique chiral outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	22	A2M	C3'	7
2	B	22	A2M	C4'	7
2	B	23	UFT	C4'	2

There are no torsion outliers.

There are no ring outliers.

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