



wwPDB NMR Structure Validation Summary Report ⓘ

Apr 27, 2016 – 06:49 AM BST

PDB ID : 2MSE
Title : NMR data-driven model of GTPase KRas-GNP:ARafRBD complex tethered to a lipid-bilayer nanodisc
Authors : Mazhab-Jafari, M.; Stathopoulos, P.; Marshall, C.; Ikura, M.
Deposited on : 2014-07-29

This is a wwPDB NMR Structure Validation Summary 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

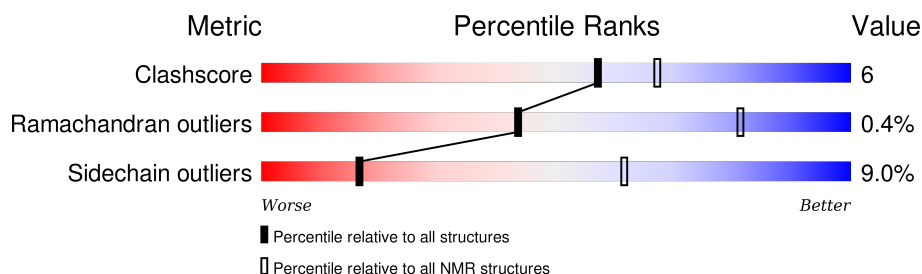
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 0%.

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	200	 64% 14% 21%
1	C	200	 80% 18%
2	B	187	 75% 16% 8%
3	D	73	 75% 25%

2 Ensemble composition and analysis

This entry contains 10 models. Model 3 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:239-A:395, C:401-C:596 (353)	0.25	3
2	B:2-B:171, D:808-D:880 (243)	0.55	5

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. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 6, 7, 8
2	4, 5, 9, 10

3 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9709 atoms, of which 64 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						Trace
1	A	198	Total	C	H	N	O	S	0
			1645	1019	22	287	314	3	
1	C	198	Total	C	H	N	O	S	0
			1646	1019	22	287	315	3	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	GLY	-	EXPRESSION TAG	UNP P02647
A	200	PRO	-	EXPRESSION TAG	UNP P02647
C	397	GLY	-	EXPRESSION TAG	UNP P02647
C	398	PRO	-	EXPRESSION TAG	UNP P02647

- Molecule 2 is a protein called V-Ki-ras2 Kirsten rat sarcoma viral oncogene homolog, isoform CRA_b.

Mol	Chain	Residues	Atoms						Trace
2	B	185	Total	C	H	N	O	S	0
			1492	923	16	257	287	9	

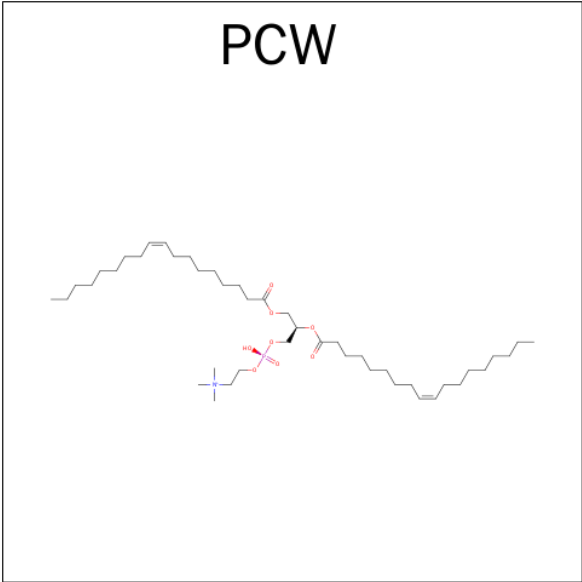
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	EXPRESSION TAG	UNP A0A024RAV5
B	0	SER	-	EXPRESSION TAG	UNP A0A024RAV5

- Molecule 3 is a protein called Serine/threonine-protein kinase A-Raf.

Mol	Chain	Residues	Atoms						Trace
3	D	73	Total	C	H	N	O	S	0
			573	360	4	99	107	3	

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C₄₄H₈₅NO₈P).



Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1

Continued on next page...

Continued from previous page...

[illegible]

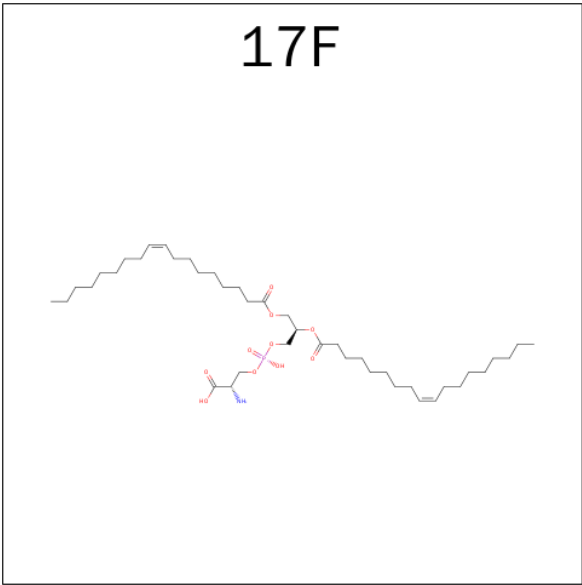
Continued on next page...

[illegible]

Continued from previous page...

Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1
4	A	1	Total	C	N	O	P
			54	44	1	8	1

- Molecule 5 is O-[(S)-({(2R)-2,3-BIS[(9Z)-OCTADEC-9-ENOYLOXY]PROPYL}OXY)(HYDROXY)PHOSPHORYL]-L-SERINE (three-letter code: 17F) (formula: C₄₂H₇₈NO₁₀P).



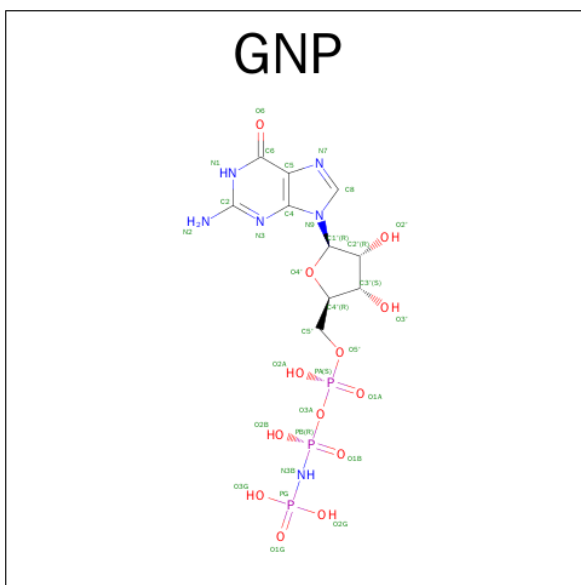
Mol	Chain	Residues	Atoms				
5	A	1	Total	C	N	O	P
			54	42	1	10	1
5	A	1	Total	C	N	O	P
			54	42	1	10	1
5	A	1	Total	C	N	O	P
			54	42	1	10	1

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				
5	A	1	Total	C	N	O	P
			54	42	1	10	1
5	A	1	Total	C	N	O	P
			54	42	1	10	1
5	A	1	Total	C	N	O	P
			54	42	1	10	1
5	A	1	Total	C	N	O	P
			54	42	1	10	1
5	A	1	Total	C	N	O	P
			54	42	1	10	1
5	A	1	Total	C	N	O	P
			54	42	1	10	1
5	A	1	Total	C	N	O	P
			54	42	1	10	1
5	A	1	Total	C	N	O	P
			54	42	1	10	1
5	A	1	Total	C	N	O	P
			54	42	1	10	1
5	A	1	Total	C	N	O	P
			54	42	1	10	1

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms				
6	B	1	Total	C	N	O	P
			32	10	6	13	3

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

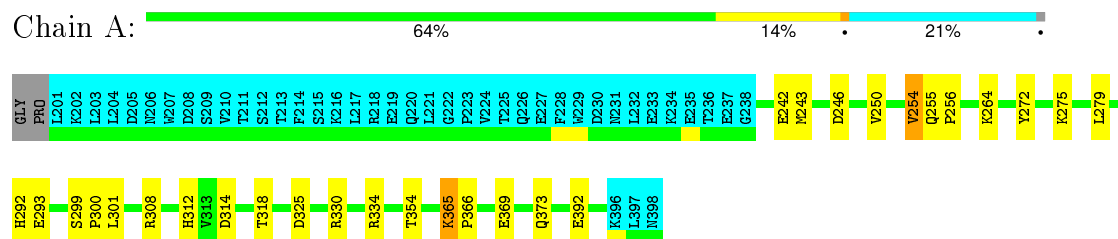
Mol	Chain	Residues	Atoms	
7	B	1	Total	Mg
			1	1

4 Residue-property plots

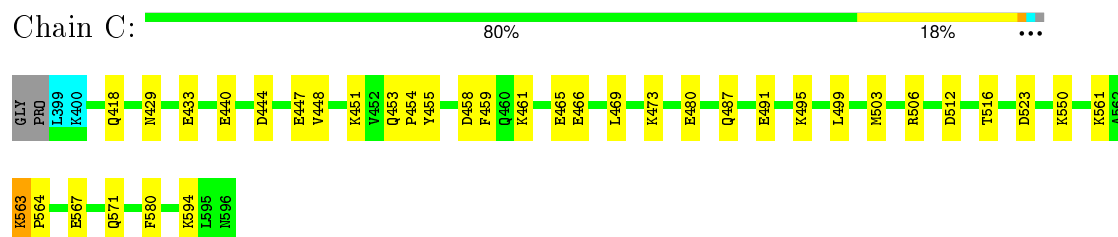
4.1 Average score per residue in the NMR ensemble

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.

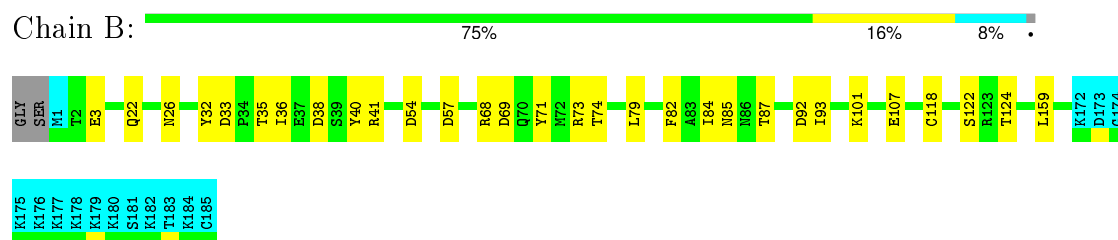
- Molecule 1: Apolipoprotein A-I



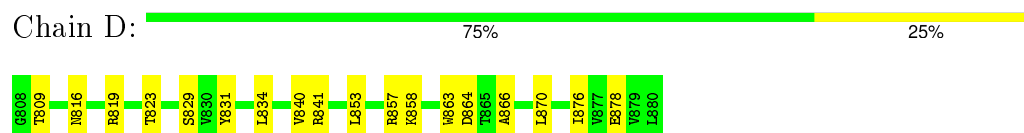
- Molecule 1: Apolipoprotein A-I



- Molecule 2: V-Ki-ras2 Kirsten rat sarcoma viral oncogene homolog, isoform CRA_b



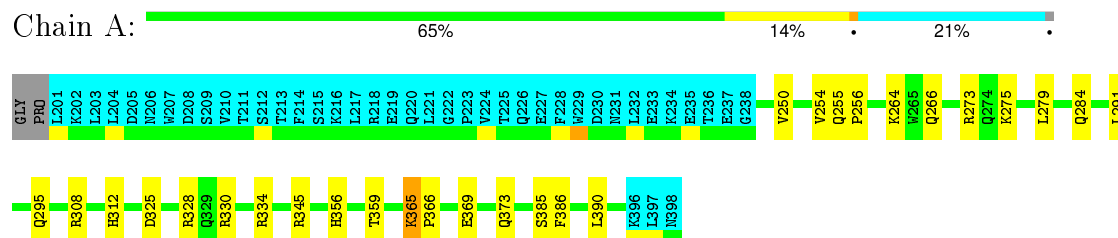
- Molecule 3: Serine/threonine-protein kinase A-Raf



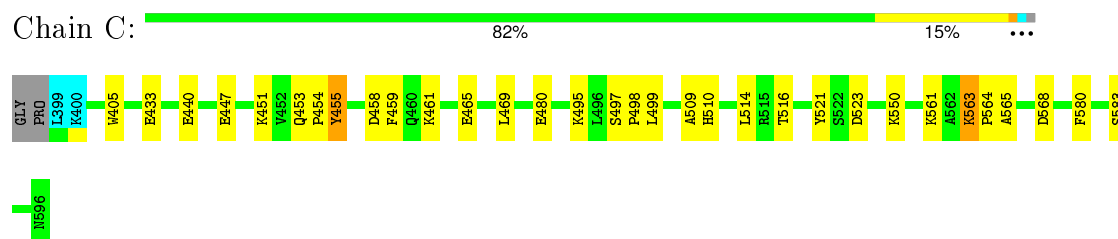
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 3. Colouring as in section 4.1 above.

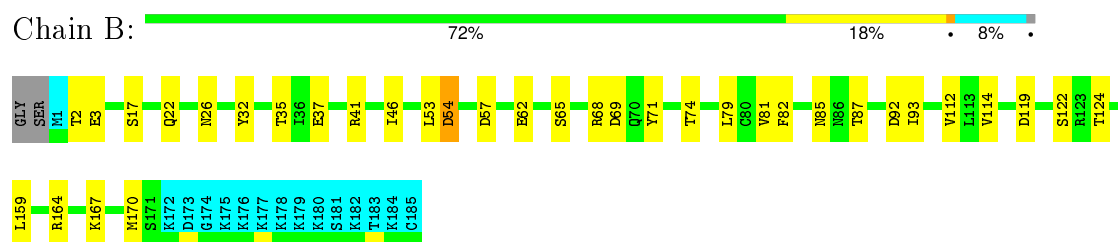
- Molecule 1: Apolipoprotein A-I



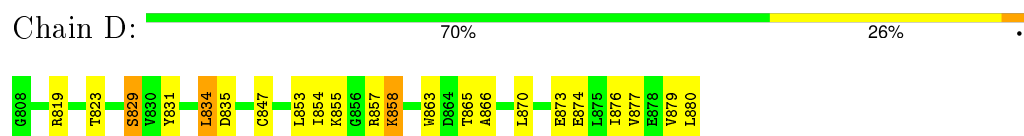
- Molecule 1: Apolipoprotein A-I



- Molecule 2: V-Ki-ras2 Kirsten rat sarcoma viral oncogene homolog, isoform CRA_b



- Molecule 3: Serine/threonine-protein kinase A-Raf



5 Refinement protocol and experimental data overview

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

Of the 3000 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
CNS	structure solution	
CHARMM-GUI	structure solution	
HADDOCK	structure solution	
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	2mse_cs.str
Number of chemical shift lists	1
Total number of shifts	52
Number of shifts mapped to atoms	52
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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: 17F, MG, GNP, PCW

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	1284	18	1297	24±6
1	C	1607	22	1603	30±6
2	B	1356	16	1336	16±5
3	D	569	4	598	15±5
4	A	3456	0	5376	60±9
5	A	864	0	1216	23±4
6	B	32	0	13	0±0
All	All	91690	600	114390	1282

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 6.

5 of 961 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:308:ARG:CD	1:C:469:LEU:HD11	1.48	1.34	1	1
1:C:465:GLU:O	1:C:469:LEU:HG	1.32	1.19	2	9
1:C:465:GLU:O	1:C:469:LEU:CG	1.26	1.82	7	6
1:A:308:ARG:CG	1:C:469:LEU:HD11	1.21	1.63	1	3
1:A:308:ARG:CD	1:C:469:LEU:CD1	1.17	2.21	1	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	157/200 (78%)	153±1 (98±1%)	3±1 (2±1%)	1±0 (1±0%)	34	78
1	C	195/200 (98%)	190±1 (98±1%)	4±2 (2±1%)	1±0 (1±0%)	38	79
2	B	170/187 (91%)	161±3 (95±2%)	9±3 (5±1%)	0±0 (0±0%)	56	85
3	D	71/73 (97%)	66±2 (93±2%)	5±2 (7±2%)	0±0 (0±0%)	59	88
All	All	5930/6600 (90%)	5702 (96%)	204 (3%)	24 (0%)	43	81

5 of 7 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	365	LYS	10
1	C	563	LYS	9
1	C	420	GLY	1
2	B	24	ILE	1
2	B	48	GLY	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	135/175 (77%)	123±3 (91±2%)	12±3 (9±2%)	17	62
1	C	172/175 (98%)	157±3 (91±2%)	15±3 (9±2%)	17	62
2	B	150/165 (91%)	137±2 (91±2%)	13±2 (9±2%)	17	62
3	D	64/64 (100%)	57±2 (89±3%)	7±2 (11±3%)	13	57
All	All	5210/5790 (90%)	4743 (91%)	467 (9%)	16	61

5 of 187 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)
3	D	819	ARG	10
2	B	87	THR	10
1	A	254	VAL	9
1	A	392	GLU	8
2	B	74	THR	8

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 82 ligands modelled in this entry, 1 is monoatomic - leaving 81 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
4	PCW	A	1	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	10	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	11	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	12	-	53,53,53	1.04±0.00	0±0 (0±0%)
4	PCW	A	13	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	14	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	15	-	53,53,53	1.04±0.00	0±0 (0±0%)
4	PCW	A	16	-	53,53,53	1.04±0.01	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PCW	A	17	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	18	-	53,53,53	1.03±0.01	0±0 (0±0%)
4	PCW	A	19	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	2	-	53,53,53	1.04±0.00	0±0 (0±0%)
4	PCW	A	20	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	21	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	22	-	53,53,53	1.03±0.01	0±0 (0±0%)
4	PCW	A	23	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	24	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	25	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	26	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	27	-	53,53,53	1.06±0.01	0±0 (0±0%)
4	PCW	A	28	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	29	-	53,53,53	1.04±0.00	0±0 (0±0%)
4	PCW	A	3	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	30	-	53,53,53	1.04±0.00	0±0 (0±0%)
4	PCW	A	31	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	32	-	53,53,53	1.04±0.01	0±0 (0±0%)
5	17F	A	33	-	50,53,53	0.92±0.01	0±0 (0±0%)
5	17F	A	34	-	50,53,53	0.92±0.00	0±0 (0±0%)
5	17F	A	35	-	50,53,53	0.92±0.01	0±0 (0±0%)
5	17F	A	36	-	50,53,53	0.92±0.01	0±0 (0±0%)
5	17F	A	37	-	50,53,53	0.92±0.01	0±0 (0±0%)
5	17F	A	38	-	50,53,53	0.91±0.00	0±0 (0±0%)
5	17F	A	39	-	50,53,53	0.92±0.00	0±0 (0±0%)
4	PCW	A	4	-	53,53,53	1.04±0.01	0±0 (0±0%)
5	17F	A	40	-	50,53,53	0.92±0.01	0±0 (0±0%)
4	PCW	A	41	-	53,53,53	1.03±0.00	0±0 (0±0%)
4	PCW	A	42	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	43	-	53,53,53	1.03±0.01	0±0 (0±0%)
4	PCW	A	44	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	45	-	53,53,53	1.04±0.00	0±0 (0±0%)
4	PCW	A	46	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	47	-	53,53,53	1.04±0.00	0±0 (0±0%)
4	PCW	A	48	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	49	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	5	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	50	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	51	-	53,53,53	1.03±0.01	0±0 (0±0%)
4	PCW	A	52	-	53,53,53	1.03±0.01	0±0 (0±0%)
4	PCW	A	53	-	53,53,53	1.04±0.00	0±0 (0±0%)
4	PCW	A	54	-	53,53,53	1.03±0.01	0±0 (0±0%)
4	PCW	A	55	-	53,53,53	1.06±0.01	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PCW	A	56	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	57	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	58	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	59	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	6	-	53,53,53	1.03±0.01	0±0 (0±0%)
4	PCW	A	60	-	53,53,53	1.04±0.00	0±0 (0±0%)
4	PCW	A	61	-	53,53,53	1.04±0.00	0±0 (0±0%)
4	PCW	A	62	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	63	-	53,53,53	1.03±0.00	0±0 (0±0%)
4	PCW	A	64	-	53,53,53	1.04±0.00	0±0 (0±0%)
4	PCW	A	65	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	66	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	67	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	68	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	69	-	53,53,53	1.04±0.00	0±0 (0±0%)
4	PCW	A	7	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	70	-	53,53,53	1.04±0.01	0±0 (0±0%)
4	PCW	A	71	-	53,53,53	1.03±0.01	0±0 (0±0%)
4	PCW	A	72	-	53,53,53	1.03±0.01	0±0 (0±0%)
5	17F	A	73	-	50,53,53	0.92±0.01	0±0 (0±0%)
5	17F	A	74	-	50,53,53	0.91±0.01	0±0 (0±0%)
5	17F	A	75	-	50,53,53	0.92±0.01	0±0 (0±0%)
5	17F	A	76	-	50,53,53	0.92±0.01	0±0 (0±0%)
5	17F	A	77	-	50,53,53	0.92±0.00	0±0 (0±0%)
5	17F	A	78	-	50,53,53	0.92±0.01	0±0 (0±0%)
5	17F	A	79	-	50,53,53	0.91±0.01	0±0 (0±0%)
4	PCW	A	8	-	53,53,53	1.04±0.01	0±0 (0±0%)
5	17F	A	80	-	50,53,53	0.92±0.01	0±0 (0±0%)
4	PCW	A	9	-	53,53,53	1.04±0.01	0±0 (0±0%)
6	GNP	B	201	-	29,34,34	1.66±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
4	PCW	A	1	-	57,61,61	2.37±0.01	3±0 (5±0%)
4	PCW	A	10	-	57,61,61	2.37±0.01	3±0 (5±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PCW	A	11	-	57,61,61	0.83±0.01	0±0 (0±0%)
4	PCW	A	12	-	57,61,61	0.83±0.01	0±0 (0±0%)
4	PCW	A	13	-	57,61,61	2.37±0.01	3±0 (5±0%)
4	PCW	A	14	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	15	-	57,61,61	0.83±0.01	0±0 (0±0%)
4	PCW	A	16	-	57,61,61	0.83±0.01	0±0 (0±0%)
4	PCW	A	17	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	18	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	19	-	57,61,61	0.83±0.01	0±0 (0±0%)
4	PCW	A	2	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	20	-	57,61,61	2.37±0.01	3±0 (5±0%)
4	PCW	A	21	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	22	-	57,61,61	2.37±0.01	3±0 (5±0%)
4	PCW	A	23	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	24	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	25	-	57,61,61	2.37±0.01	3±0 (5±0%)
4	PCW	A	26	-	57,61,61	2.37±0.01	3±0 (5±0%)
4	PCW	A	27	-	57,61,61	0.81±0.01	0±0 (0±0%)
4	PCW	A	28	-	57,61,61	2.37±0.01	3±0 (5±0%)
4	PCW	A	29	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	3	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	30	-	57,61,61	0.84±0.01	0±0 (0±0%)
4	PCW	A	31	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	32	-	57,61,61	0.83±0.00	0±0 (0±0%)
5	17F	A	33	-	50,60,60	1.74±0.02	2±0 (4±0%)
5	17F	A	34	-	50,60,60	1.00±0.03	0±0 (0±0%)
5	17F	A	35	-	50,60,60	1.00±0.02	0±0 (0±0%)
5	17F	A	36	-	50,60,60	1.00±0.02	0±0 (0±0%)
5	17F	A	37	-	50,60,60	0.98±0.02	0±0 (0±0%)
5	17F	A	38	-	50,60,60	1.00±0.03	0±0 (0±0%)
5	17F	A	39	-	50,60,60	1.00±0.02	0±0 (0±0%)
4	PCW	A	4	-	57,61,61	2.37±0.00	3±0 (5±0%)
5	17F	A	40	-	50,60,60	0.99±0.04	0±0 (0±0%)
4	PCW	A	41	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	42	-	57,61,61	2.37±0.01	3±0 (5±0%)
4	PCW	A	43	-	57,61,61	2.37±0.01	3±0 (5±0%)
4	PCW	A	44	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	45	-	57,61,61	2.37±0.00	3±0 (5±0%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
4	PCW	A	46	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	47	-	57,61,61	0.83±0.01	0±0 (0±0%)
4	PCW	A	48	-	57,61,61	0.83±0.01	0±0 (0±0%)
4	PCW	A	49	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	5	-	57,61,61	2.37±0.01	3±0 (5±0%)
4	PCW	A	50	-	57,61,61	0.83±0.01	0±0 (0±0%)
4	PCW	A	51	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	52	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	53	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	54	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	55	-	57,61,61	0.82±0.01	0±0 (0±0%)
4	PCW	A	56	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	57	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	58	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	59	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	6	-	57,61,61	2.78±0.00	6±0 (10±0%)
4	PCW	A	60	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	61	-	57,61,61	2.37±0.01	3±0 (5±0%)
4	PCW	A	62	-	57,61,61	2.37±0.01	3±0 (5±0%)
4	PCW	A	63	-	57,61,61	2.78±0.00	6±0 (10±0%)
4	PCW	A	64	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	65	-	57,61,61	0.83±0.00	0±0 (0±0%)
4	PCW	A	66	-	57,61,61	0.83±0.01	0±0 (0±0%)
4	PCW	A	67	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	68	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	69	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	7	-	57,61,61	0.83±0.01	0±0 (0±0%)
4	PCW	A	70	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	71	-	57,61,61	2.37±0.00	3±0 (5±0%)
4	PCW	A	72	-	57,61,61	0.83±0.00	0±0 (0±0%)
5	17F	A	73	-	50,60,60	1.00±0.04	0±0 (0±0%)
5	17F	A	74	-	50,60,60	0.98±0.03	0±0 (0±0%)
5	17F	A	75	-	50,60,60	1.00±0.02	0±0 (0±0%)
5	17F	A	76	-	50,60,60	0.96±0.02	0±0 (0±0%)
5	17F	A	77	-	50,60,60	1.72±0.02	2±0 (4±0%)
5	17F	A	78	-	50,60,60	0.98±0.03	0±0 (0±0%)
5	17F	A	79	-	50,60,60	1.02±0.02	0±0 (0±0%)
4	PCW	A	8	-	57,61,61	0.83±0.01	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
5	17F	A	80	-	50,60,60	0.95±0.02	0±0 (0±0%)
4	PCW	A	9	-	57,61,61	0.82±0.01	0±0 (0±0%)
6	GNP	B	201	-	29,54,54	2.46±0.02	2±0 (6±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
4	PCW	A	1	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	10	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	11	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	12	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	13	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	14	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	15	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	16	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	17	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	18	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	19	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	2	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	20	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	21	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	22	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	23	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	24	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	25	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	26	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	27	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	28	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	29	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	3	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	30	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	31	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	32	-	-	0±0,57,57,57	0±0,0,0,0
5	17F	A	33	-	-	0±0,55,59,59	0±0,0,0,0
5	17F	A	34	-	-	0±0,55,59,59	0±0,0,0,0
5	17F	A	35	-	-	0±0,55,59,59	0±0,0,0,0
5	17F	A	36	-	-	0±0,55,59,59	0±0,0,0,0
5	17F	A	37	-	-	0±0,55,59,59	0±0,0,0,0
5	17F	A	38	-	-	0±0,55,59,59	0±0,0,0,0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	17F	A	39	-	-	0±0,55,59,59	0±0,0,0,0
4	PCW	A	4	-	-	0±0,57,57,57	0±0,0,0,0
5	17F	A	40	-	-	0±0,55,59,59	0±0,0,0,0
4	PCW	A	41	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	42	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	43	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	44	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	45	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	46	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	47	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	48	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	49	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	5	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	50	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	51	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	52	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	53	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	54	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	55	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	56	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	57	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	58	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	59	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	6	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	60	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	61	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	62	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	63	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	64	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	65	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	66	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	67	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	68	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	69	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	7	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	70	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	71	-	-	0±0,57,57,57	0±0,0,0,0
4	PCW	A	72	-	-	0±0,57,57,57	0±0,0,0,0
5	17F	A	73	-	-	0±0,55,59,59	0±0,0,0,0
5	17F	A	74	-	-	0±0,55,59,59	0±0,0,0,0
5	17F	A	75	-	-	0±0,55,59,59	0±0,0,0,0
5	17F	A	76	-	-	0±0,55,59,59	0±0,0,0,0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	17F	A	77	-	-	0±0,55,59,59	0±0,0,0,0
5	17F	A	78	-	-	0±0,55,59,59	0±0,0,0,0
5	17F	A	79	-	-	0±0,55,59,59	0±0,0,0,0
4	PCW	A	8	-	-	0±0,57,57,57	0±0,0,0,0
5	17F	A	80	-	-	0±0,55,59,59	0±0,0,0,0
4	PCW	A	9	-	-	0±0,57,57,57	0±0,0,0,0
6	GNP	B	201	-	-	0±0,13,38,38	0±0,3,3,3

There are no bond-length outliers.

5 of 150 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
4	A	28	PCW	C8-N-C7	12.22	77.35	108.96	3	10
4	A	56	PCW	C8-N-C7	12.16	77.49	108.96	2	10
4	A	10	PCW	C8-N-C7	12.15	77.54	108.96	10	10
4	A	64	PCW	C8-N-C7	12.13	77.57	108.96	9	10
4	A	13	PCW	C8-N-C7	12.13	77.57	108.96	10	10

There are no chirality outliers.

All unique torsion outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
5	A	74	17F	C5-O9-C17-C18	1

There are no ring outliers.

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](#)

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: 2mse_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	52
Number of shifts mapped to atoms	52
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 26 atoms were assigned a chemical shift out of a possible 7601. 0 out of 118 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/2942 (0%)	0/1173 (0%)	0/1192 (0%)	0/577 (0%)
Sidechain	26/4226 (1%)	13/2472 (1%)	13/1535 (1%)	0/219 (0%)
Aromatic	0/433 (0%)	0/240 (0%)	0/193 (0%)	0/0 (—%)
Overall	26/7601 (0%)	13/3885 (0%)	13/2920 (0%)	0/796 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.