



# wwPDB NMR Structure Validation Summary Report ⓘ

Feb 13, 2017 – 04:59 am GMT

PDB ID : 2MZI  
Title : NMR Solution Structure of the PRO Form of Human Matrilysin (proMMP-7)  
in Complex with Anionic Membrane  
Authors : Prior, S.H.; Van Doren, S.R.  
Deposited on : 2015-02-12

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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	:	1.7.2 (RC1), CSD as538be (2017)
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

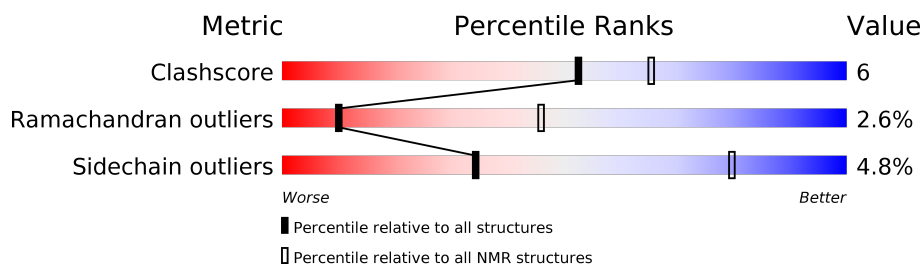
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*


The overall completeness of chemical shifts assignment is 21%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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  $\geq 3$ , 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	250	

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
5	A	C3S	431	20	-
5	A	C3S	432	20	-
5	A	C3S	433	20	-
5	A	C3S	434	20	-
5	A	C3S	435	20	-
5	A	C3S	436	20	-

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:2-A:75, A:82-A:244 (237)	0.69	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 3 clusters. No single-model clusters were found.

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

### 3 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10109 atoms, of which 2165 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Matrilysin.

Mol	Chain	Residues	Atoms						Trace
1	A	248	Total	C	H	N	O	S	0
			3847	1240	1895	339	364	9	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	ALA	GLU	ENGINEERED MUTATION	UNP P09237

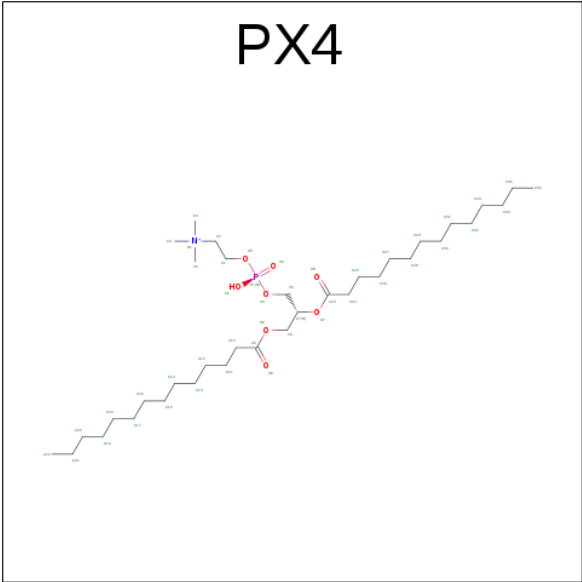
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Ca
			2	2

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
3	A	2	Total	Zn
			2	2

- Molecule 4 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C<sub>36</sub>H<sub>73</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1

Continued on next page...

[illegible]

[illegible]

*Continued from previous page...*

Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1

*Continued on next page...*



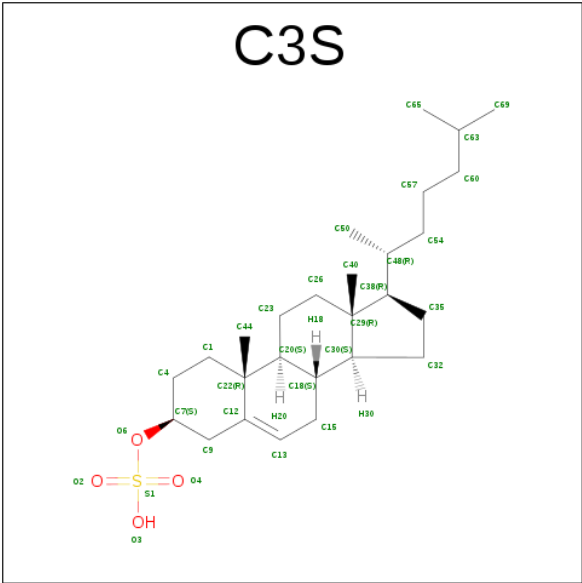
[illegible]

[illegible]

Continued from previous page...

Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1

- Molecule 5 is CHOLEST-5-EN-3-YL HYDROGEN SULFATE (three-letter code: C3S) (formula: C<sub>27</sub>H<sub>46</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms				
5	A	1	Total	C	H	O	S
			77	27	45	4	1
5	A	1	Total	C	H	O	S
			77	27	45	4	1
5	A	1	Total	C	H	O	S
			77	27	45	4	1
5	A	1	Total	C	H	O	S
			77	27	45	4	1

Continued on next page...

*Continued from previous page...*

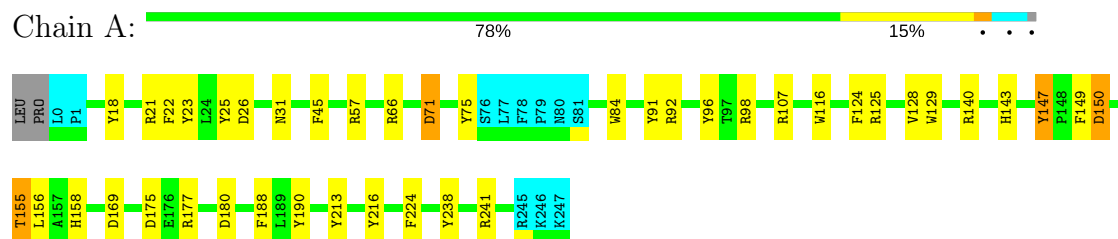
Mol	Chain	Residues	Atoms				
5	A	1	Total	C	H	O	S
			77	27	45	4	1
5	A	1	Total	C	H	O	S
			77	27	45	4	1

## 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.

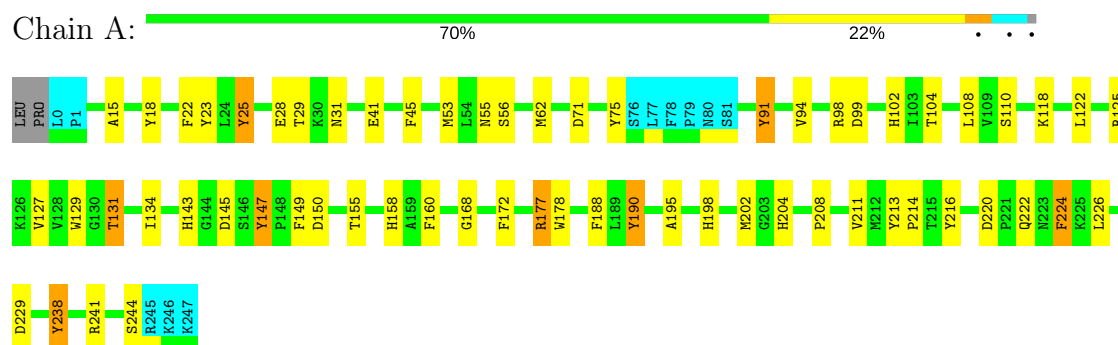
- Molecule 1: Matrilysin



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

The representative model is number 5. Colouring as in section 4.1 above.

- Molecule 1: Matrilysin



## 5 Refinement protocol and experimental data overview

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

Of the 10000 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
HADDOCK	structure solution	2.1
GROMOS	refinement	4.5.7

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)	2mzi_cs.str
Number of chemical shift lists	1
Total number of shifts	797
Number of shifts mapped to atoms	797
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	21%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 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: ZN, CA, C3S, PX4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.52±0.00	0±0/1912 (0.0±0.0%)	2.02±0.04	56±8/2587 (2.2±0.3%)
All	All	0.52	0/38240 (0.0%)	2.02	1128/51740 (2.2%)

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	7.2±2.1
All	All	0	144

There are no bond-length outliers.

5 of 456 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
1	A	177	ARG	NE-CZ-NH2	-19.51	110.54	120.30	5	12
1	A	140	ARG	NE-CZ-NH2	-18.98	110.81	120.30	14	12
1	A	140	ARG	NE-CZ-NH1	18.27	129.44	120.30	1	8
1	A	125	ARG	NE-CZ-NH2	-17.59	111.51	120.30	2	11
1	A	57	ARG	NE-CZ-NH2	-17.59	111.51	120.30	1	8

There are no chirality outliers.

5 of 60 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	238	TYR	Sidechain	11

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group	Models (Total)
1	A	18	TYR	Sidechain	8
1	A	96	TYR	Sidechain	7
1	A	190	TYR	Sidechain	7
1	A	149	PHE	Sidechain,Peptide	6

## 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	1861	1796	1796	4±2
4	A	5796	0	9072	122±10
5	A	192	270	272	3±2
All	All	157060	41320	222802	2459

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 2410 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:384:PX4:H50	4:A:427:PX4:H60	0.91	1.43	1	1
4:A:328:PX4:H39	4:A:351:PX4:H23	0.90	1.41	12	1
4:A:386:PX4:H42	4:A:417:PX4:H38	0.85	1.47	3	1
4:A:308:PX4:H17	4:A:326:PX4:H55	0.84	1.49	15	1
4:A:367:PX4:H16	4:A:399:PX4:H47	0.84	1.48	17	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	237/250 (95%)	211±3 (89±1%)	20±3 (8±1%)	6±1 (3±1%)	10	46
All	All	4740/5000 (95%)	4216 (89%)	401 (8%)	123 (3%)	10	46

5 of 22 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	31	ASN	18
1	A	147	TYR	18
1	A	150	ASP	16
1	A	224	PHE	11
1	A	25	TYR	11

### 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	195/208 (94%)	186±3 (95±2%)	9±3 (5±2%)	34	79
All	All	3900/4160 (94%)	3711 (95%)	189 (5%)	34	79

5 of 68 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	150	ASP	20
1	A	155	THR	12
1	A	158	HIS	9
1	A	177	ARG	9
1	A	75	TYR	8

### 6.3.3 RNA ⓘ

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 136 ligands modelled in this entry, 4 are monoatomic - leaving 132 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	PX4	A	305	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	306	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	307	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	308	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	309	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	310	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	311	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	312	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	313	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	314	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	315	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	316	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	317	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	318	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	319	-	45,45,45	0.62±0.01	0±0 (0±0%)
4	PX4	A	320	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	321	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	322	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	323	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	324	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	325	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	326	-	45,45,45	0.62±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	327	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	328	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	329	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	330	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	331	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	332	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	333	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	334	-	45,45,45	0.62±0.01	0±0 (0±0%)
4	PX4	A	335	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	336	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	337	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	338	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	339	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	340	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	341	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	342	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	343	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	344	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	345	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	346	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	347	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	348	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	349	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	350	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	351	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	352	-	45,45,45	0.62±0.01	0±0 (0±0%)
4	PX4	A	353	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	354	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	355	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	356	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	357	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	358	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	359	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	360	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	361	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	362	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	363	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	364	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	365	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	366	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	367	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	368	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	369	-	45,45,45	0.62±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	370	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	371	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	372	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	373	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	374	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	375	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	376	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	377	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	378	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	379	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	380	-	45,45,45	0.62±0.01	0±0 (0±0%)
4	PX4	A	381	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	382	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	383	-	45,45,45	0.62±0.01	0±0 (0±0%)
4	PX4	A	384	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	385	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	386	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	387	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	388	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	389	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	390	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	391	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	392	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	393	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	394	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	395	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	396	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	397	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	398	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	399	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	400	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	401	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	402	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	403	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	404	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	405	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	406	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	407	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	408	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	409	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	410	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	411	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	412	-	45,45,45	0.63±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	413	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	414	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	415	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	416	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	417	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	418	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	419	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	420	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	421	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	422	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	423	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	424	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	425	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	426	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	427	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	428	-	45,45,45	0.63±0.00	0±0 (0±0%)
4	PX4	A	429	-	45,45,45	0.62±0.00	0±0 (0±0%)
4	PX4	A	430	-	45,45,45	0.62±0.00	0±0 (0±0%)
5	C3S	A	431	-	35,35,35	1.34±0.01	1±0 (2±0%)
5	C3S	A	432	-	35,35,35	1.34±0.01	1±0 (2±0%)
5	C3S	A	433	-	35,35,35	1.34±0.01	1±0 (2±0%)
5	C3S	A	434	-	35,35,35	1.35±0.01	1±0 (2±0%)
5	C3S	A	435	-	35,35,35	1.34±0.01	1±0 (2±0%)
5	C3S	A	436	-	35,35,35	1.34±0.01	1±0 (2±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	PX4	A	305	-	50,53,53	1.44±0.10	0±0 (0±0%)
4	PX4	A	306	-	50,53,53	1.53±0.13	0±0 (0±0%)
4	PX4	A	307	-	50,53,53	1.49±0.15	0±0 (0±0%)
4	PX4	A	308	-	50,53,53	1.48±0.17	0±0 (0±0%)
4	PX4	A	309	-	50,53,53	1.54±0.17	0±1 (0±1%)
4	PX4	A	310	-	50,53,53	1.50±0.17	0±1 (0±1%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	311	-	50,53,53	1.49±0.16	0±1 (0±1%)
4	PX4	A	312	-	50,53,53	1.47±0.18	0±1 (0±1%)
4	PX4	A	313	-	50,53,53	1.48±0.15	0±0 (0±0%)
4	PX4	A	314	-	50,53,53	1.49±0.14	0±0 (0±0%)
4	PX4	A	315	-	50,53,53	1.43±0.12	0±0 (0±0%)
4	PX4	A	316	-	50,53,53	1.48±0.13	0±1 (0±1%)
4	PX4	A	317	-	50,53,53	1.43±0.17	0±0 (0±0%)
4	PX4	A	318	-	50,53,53	1.50±0.14	0±0 (0±0%)
4	PX4	A	319	-	50,53,53	1.51±0.18	0±1 (0±1%)
4	PX4	A	320	-	50,53,53	1.49±0.14	0±0 (0±0%)
4	PX4	A	321	-	50,53,53	1.48±0.13	0±0 (0±0%)
4	PX4	A	322	-	50,53,53	1.53±0.14	0±0 (0±0%)
4	PX4	A	323	-	50,53,53	1.50±0.11	0±0 (0±0%)
4	PX4	A	324	-	50,53,53	1.50±0.17	0±0 (0±0%)
4	PX4	A	325	-	50,53,53	1.52±0.17	0±0 (0±0%)
4	PX4	A	326	-	50,53,53	1.51±0.15	0±0 (0±0%)
4	PX4	A	327	-	50,53,53	1.40±0.18	0±0 (0±0%)
4	PX4	A	328	-	50,53,53	1.55±0.19	0±0 (0±0%)
4	PX4	A	329	-	50,53,53	1.43±0.14	0±0 (0±0%)
4	PX4	A	330	-	50,53,53	1.55±0.13	0±1 (0±1%)
4	PX4	A	331	-	50,53,53	1.53±0.17	0±0 (0±0%)
4	PX4	A	332	-	50,53,53	1.49±0.15	0±0 (0±0%)
4	PX4	A	333	-	50,53,53	1.47±0.21	0±0 (0±0%)
4	PX4	A	334	-	50,53,53	1.48±0.14	0±0 (0±0%)
4	PX4	A	335	-	50,53,53	1.54±0.15	0±0 (0±0%)
4	PX4	A	336	-	50,53,53	1.55±0.20	0±0 (0±0%)
4	PX4	A	337	-	50,53,53	1.47±0.16	0±0 (0±0%)
4	PX4	A	338	-	50,53,53	1.48±0.20	0±0 (0±0%)
4	PX4	A	339	-	50,53,53	1.41±0.13	0±0 (0±0%)
4	PX4	A	340	-	50,53,53	1.49±0.15	0±0 (0±0%)
4	PX4	A	341	-	50,53,53	1.48±0.20	0±0 (0±0%)
4	PX4	A	342	-	50,53,53	1.49±0.17	0±0 (0±0%)
4	PX4	A	343	-	50,53,53	1.56±0.16	0±0 (0±0%)
4	PX4	A	344	-	50,53,53	1.43±0.19	0±0 (0±0%)
4	PX4	A	345	-	50,53,53	1.49±0.17	0±1 (0±1%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	346	-	50,53,53	1.50±0.15	0±0 (0±0%)
4	PX4	A	347	-	50,53,53	1.52±0.15	0±0 (0±0%)
4	PX4	A	348	-	50,53,53	1.49±0.12	0±0 (0±0%)
4	PX4	A	349	-	50,53,53	1.47±0.13	0±1 (0±1%)
4	PX4	A	350	-	50,53,53	1.46±0.13	0±0 (0±0%)
4	PX4	A	351	-	50,53,53	1.44±0.15	0±0 (0±0%)
4	PX4	A	352	-	50,53,53	1.50±0.12	0±0 (0±0%)
4	PX4	A	353	-	50,53,53	1.53±0.20	0±1 (0±1%)
4	PX4	A	354	-	50,53,53	1.52±0.20	0±0 (0±0%)
4	PX4	A	355	-	50,53,53	1.48±0.16	0±1 (0±1%)
4	PX4	A	356	-	50,53,53	1.56±0.16	0±0 (0±0%)
4	PX4	A	357	-	50,53,53	1.57±0.16	0±0 (0±0%)
4	PX4	A	358	-	50,53,53	1.45±0.19	0±0 (0±0%)
4	PX4	A	359	-	50,53,53	1.50±0.13	0±0 (0±0%)
4	PX4	A	360	-	50,53,53	1.48±0.17	0±0 (0±0%)
4	PX4	A	361	-	50,53,53	1.47±0.19	0±1 (0±1%)
4	PX4	A	362	-	50,53,53	1.43±0.13	0±0 (0±0%)
4	PX4	A	363	-	50,53,53	1.45±0.17	0±0 (0±0%)
4	PX4	A	364	-	50,53,53	1.50±0.15	0±0 (0±0%)
4	PX4	A	365	-	50,53,53	1.48±0.15	0±0 (0±0%)
4	PX4	A	366	-	50,53,53	1.41±0.16	0±0 (0±0%)
4	PX4	A	367	-	50,53,53	1.50±0.14	0±1 (0±1%)
4	PX4	A	368	-	50,53,53	1.47±0.11	0±0 (0±0%)
4	PX4	A	369	-	50,53,53	1.45±0.08	0±0 (0±0%)
4	PX4	A	370	-	50,53,53	1.49±0.15	0±0 (0±0%)
4	PX4	A	371	-	50,53,53	1.51±0.13	0±0 (0±0%)
4	PX4	A	372	-	50,53,53	1.52±0.21	0±1 (0±1%)
4	PX4	A	373	-	50,53,53	1.47±0.18	0±0 (0±0%)
4	PX4	A	374	-	50,53,53	1.47±0.15	0±0 (0±0%)
4	PX4	A	375	-	50,53,53	1.52±0.16	0±0 (0±0%)
4	PX4	A	376	-	50,53,53	1.55±0.23	0±1 (0±1%)
4	PX4	A	377	-	50,53,53	1.50±0.15	0±0 (0±0%)
4	PX4	A	378	-	50,53,53	1.49±0.20	0±0 (0±0%)
4	PX4	A	379	-	50,53,53	1.50±0.15	0±0 (0±0%)
4	PX4	A	380	-	50,53,53	1.46±0.13	0±0 (0±0%)



Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	381	-	50,53,53	1.56±0.18	0±1 (0±1%)
4	PX4	A	382	-	50,53,53	1.49±0.10	0±0 (0±0%)
4	PX4	A	383	-	50,53,53	1.46±0.17	0±0 (0±0%)
4	PX4	A	384	-	50,53,53	1.52±0.17	0±0 (0±0%)
4	PX4	A	385	-	50,53,53	1.49±0.14	0±0 (0±0%)
4	PX4	A	386	-	50,53,53	1.49±0.12	0±0 (0±0%)
4	PX4	A	387	-	50,53,53	1.54±0.12	0±0 (0±0%)
4	PX4	A	388	-	50,53,53	1.45±0.11	0±0 (0±0%)
4	PX4	A	389	-	50,53,53	1.48±0.14	0±0 (0±0%)
4	PX4	A	390	-	50,53,53	1.48±0.13	0±0 (0±0%)
4	PX4	A	391	-	50,53,53	1.46±0.13	0±0 (0±0%)
4	PX4	A	392	-	50,53,53	1.50±0.13	0±1 (0±1%)
4	PX4	A	393	-	50,53,53	1.52±0.14	0±1 (0±1%)
4	PX4	A	394	-	50,53,53	1.49±0.16	0±0 (0±0%)
4	PX4	A	395	-	50,53,53	1.52±0.17	0±0 (0±0%)
4	PX4	A	396	-	50,53,53	1.45±0.14	0±0 (0±0%)
4	PX4	A	397	-	50,53,53	1.52±0.13	0±0 (0±0%)
4	PX4	A	398	-	50,53,53	1.48±0.15	0±0 (0±0%)
4	PX4	A	399	-	50,53,53	1.51±0.16	0±0 (0±0%)
4	PX4	A	400	-	50,53,53	1.46±0.15	0±0 (0±0%)
4	PX4	A	401	-	50,53,53	1.55±0.18	0±1 (0±1%)
4	PX4	A	402	-	50,53,53	1.54±0.16	0±1 (0±1%)
4	PX4	A	403	-	50,53,53	1.47±0.11	0±0 (0±0%)
4	PX4	A	404	-	50,53,53	1.42±0.15	0±0 (0±0%)
4	PX4	A	405	-	50,53,53	1.55±0.15	0±0 (0±0%)
4	PX4	A	406	-	50,53,53	1.47±0.15	0±0 (0±0%)
4	PX4	A	407	-	50,53,53	1.49±0.16	0±0 (0±0%)
4	PX4	A	408	-	50,53,53	1.48±0.22	0±1 (0±1%)
4	PX4	A	409	-	50,53,53	1.55±0.16	0±0 (0±0%)
4	PX4	A	410	-	50,53,53	1.45±0.10	0±0 (0±0%)
4	PX4	A	411	-	50,53,53	1.50±0.17	0±0 (0±0%)
4	PX4	A	412	-	50,53,53	1.47±0.18	0±0 (0±0%)
4	PX4	A	413	-	50,53,53	1.50±0.16	0±0 (0±0%)
4	PX4	A	414	-	50,53,53	1.49±0.13	0±0 (0±0%)
4	PX4	A	415	-	50,53,53	1.51±0.14	0±0 (0±0%)



Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	416	-	50,53,53	1.52±0.16	0±1 (0±1%)
4	PX4	A	417	-	50,53,53	1.50±0.15	0±0 (0±0%)
4	PX4	A	418	-	50,53,53	1.55±0.17	0±0 (0±0%)
4	PX4	A	419	-	50,53,53	1.55±0.14	0±0 (0±0%)
4	PX4	A	420	-	50,53,53	1.48±0.13	0±0 (0±0%)
4	PX4	A	421	-	50,53,53	1.51±0.18	0±1 (0±1%)
4	PX4	A	422	-	50,53,53	1.45±0.14	0±0 (0±0%)
4	PX4	A	423	-	50,53,53	1.47±0.16	0±0 (0±0%)
4	PX4	A	424	-	50,53,53	1.45±0.20	0±0 (0±0%)
4	PX4	A	425	-	50,53,53	1.47±0.15	0±0 (0±0%)
4	PX4	A	426	-	50,53,53	1.43±0.17	0±0 (0±0%)
4	PX4	A	427	-	50,53,53	1.49±0.19	0±0 (0±0%)
4	PX4	A	428	-	50,53,53	1.43±0.18	0±0 (0±0%)
4	PX4	A	429	-	50,53,53	1.49±0.14	0±0 (0±0%)
4	PX4	A	430	-	50,53,53	1.40±0.18	0±0 (0±0%)
5	C3S	A	431	-	51,55,55	2.25±0.30	1±1 (2±1%)
5	C3S	A	432	-	51,55,55	2.34±0.21	2±1 (4±2%)
5	C3S	A	433	-	51,55,55	2.24±0.21	1±1 (2±1%)
5	C3S	A	434	-	51,55,55	2.24±0.25	1±1 (2±2%)
5	C3S	A	435	-	51,55,55	2.25±0.20	1±1 (2±2%)
5	C3S	A	436	-	51,55,55	2.28±0.23	2±1 (3±2%)

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	PX4	A	305	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	306	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	307	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	308	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	309	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	310	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	311	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	312	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	313	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	314	-	-	0±0,49,49,49	0±0,0,0,0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	315	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	316	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	317	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	318	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	319	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	320	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	321	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	322	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	323	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	324	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	325	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	326	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	327	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	328	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	329	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	330	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	331	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	332	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	333	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	334	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	335	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	336	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	337	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	338	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	339	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	340	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	341	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	342	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	343	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	344	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	345	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	346	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	347	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	348	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	349	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	350	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	351	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	352	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	353	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	354	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	355	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	356	-	-	2±0,49,49,49	0±0,0,0,0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	357	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	358	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	359	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	360	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	361	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	362	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	363	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	364	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	365	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	366	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	367	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	368	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	369	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	370	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	371	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	372	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	373	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	374	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	375	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	376	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	377	-	-	2±0,49,49,49	0±0,0,0,0
4	PX4	A	378	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	379	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	380	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	381	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	382	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	383	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	384	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	385	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	386	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	387	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	388	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	389	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	390	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	391	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	392	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	393	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	394	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	395	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	396	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	397	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	398	-	-	0±0,49,49,49	0±0,0,0,0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	399	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	400	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	401	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	402	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	403	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	404	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	405	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	406	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	407	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	408	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	409	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	410	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	411	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	412	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	413	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	414	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	415	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	416	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	417	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	418	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	419	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	420	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	421	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	422	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	423	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	424	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	425	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	426	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	427	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	428	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	429	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	430	-	-	0±0,49,49,49	0±0,0,0,0
5	C3S	A	431	-	2±0,2,12,12	0±0,15,73,73	0±0,4,4,4
5	C3S	A	432	-	1±0,1,12,12	0±0,15,73,73	0±0,4,4,4
5	C3S	A	433	-	1±0,1,12,12	0±0,15,73,73	0±0,4,4,4
5	C3S	A	434	-	1±0,1,12,12	0±0,15,73,73	0±0,4,4,4
5	C3S	A	435	-	2±0,2,12,12	0±0,15,73,73	0±0,4,4,4
5	C3S	A	436	-	2±0,2,12,12	0±0,15,73,73	0±0,4,4,4

5 of 6 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
5	A	434	C3S	O6-S1	6.81	1.76	1.56	7	20
5	A	435	C3S	O6-S1	6.79	1.76	1.56	14	20
5	A	432	C3S	O6-S1	6.79	1.76	1.56	3	20
5	A	436	C3S	O6-S1	6.79	1.76	1.56	7	20
5	A	433	C3S	O6-S1	6.78	1.76	1.56	12	20

5 of 404 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
5	A	432	C3S	C29-C38-C48	10.05	135.60	119.47	14	14
5	A	433	C3S	O6-C7-C4	9.16	121.32	107.54	20	2
5	A	434	C3S	C29-C38-C48	9.13	134.12	119.47	15	5
5	A	436	C3S	C50-C48-C38	8.57	126.36	112.95	16	5
4	A	375	PX4	C8-C7-C6	8.49	92.71	111.86	11	1

5 of 9 unique chiral outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
5	A	431	C3S	C7	20
5	A	431	C3S	C48	20
5	A	433	C3S	C48	20
5	A	435	C3S	C7	20
5	A	435	C3S	C48	20

5 of 10 unique torsion outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Models (Total)
4	A	377	PX4	C7-O7-C23-O8	14
4	A	377	PX4	C7-O7-C23-C24	14
4	A	376	PX4	C7-O7-C23-O8	5
4	A	376	PX4	C7-O7-C23-C24	5
4	A	356	PX4	C7-O7-C23-O8	3

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

The completeness of assignment taking into account all chemical shift lists is 21% for the well-defined parts and 20% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2mzi\_cs.str

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

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	797
Number of shifts mapped to atoms	797
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	188	$0.12 \pm 0.20$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 21%, i.e. 605 atoms were assigned a chemical shift out of a possible 2874. 10 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	417/1161 (36%)	233/462 (50%)	0/474 (0%)	184/225 (82%)
Sidechain	175/1419 (12%)	126/838 (15%)	45/517 (9%)	4/64 (6%)

*Continued on next page...*

Continued from previous page...

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Aromatic	13/294 (4%)	9/156 (6%)	0/125 (0%)	4/13 (31%)
Overall	605/2874 (21%)	368/1456 (25%)	45/1116 (4%)	192/302 (64%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

