



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2MLR  
Title : Membrane Bilayer complex with Matrix Metalloproteinase-12 at its Alpha-face  
Authors : Koppiseti, R.K.; Fulcher, Y.G.; Prior, S.H.; Lenoir, M.; Overduin, M.; Van Doren, S.R.  
Deposited on : 2014-03-04

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.

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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

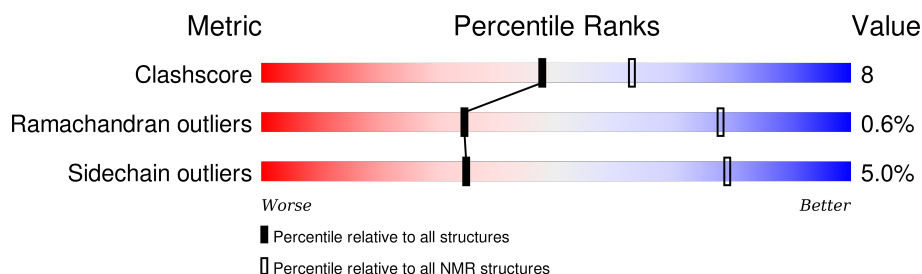
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 83%.

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  $\geq 3$ , 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	164	 79% 18% ..

## 2 Ensemble composition and analysis ⓘ

This entry contains 14 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:100-A:187, A:192-A:263 (160)	0.38	3

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 4 clusters. No single-model clusters were found.

Cluster number	Models
1	8, 9, 10, 11, 13
2	1, 2, 3, 4, 5
3	6, 7
4	12, 14

### 3 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8263 atoms, of which 1221 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Macrophage metalloelastase.

Mol	Chain	Residues	Atoms						Trace
1	A	164	Total	C	H	N	O	S	0
			2508	824	1221	225	234	4	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	ALA	GLU	ENGINEERED MUTATION	UNP P39900

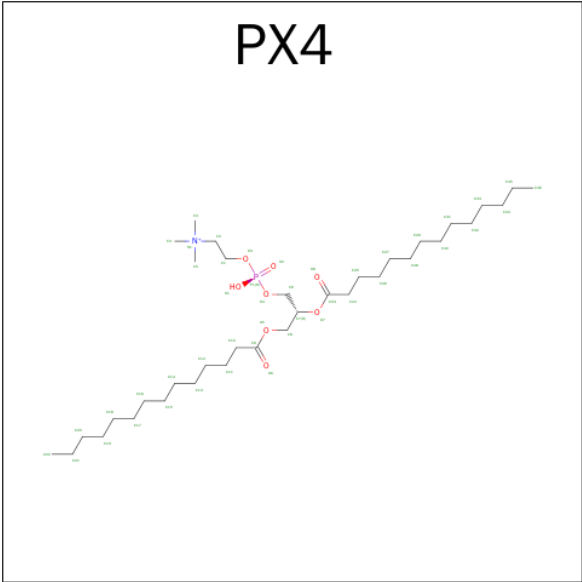
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
3	A	3	Total	Ca
			3	3

- 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

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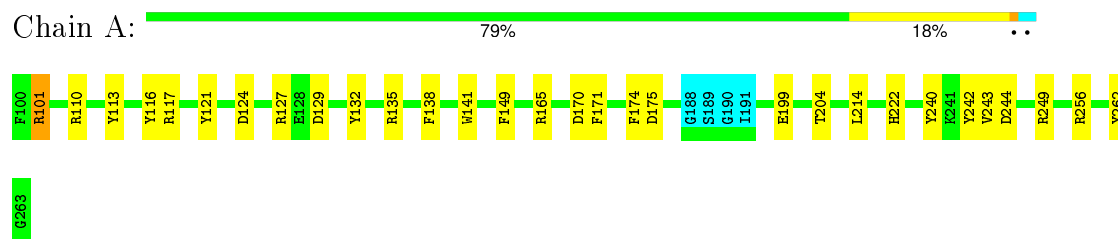
Mol	Chain	Residues	Atoms				
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1
4	A	1	Total	C	N	O	P
			46	36	1	8	1

## 4 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.

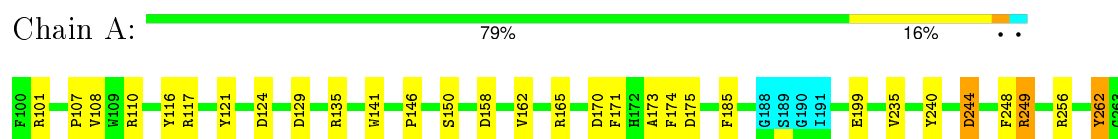
- Molecule 1: Macrophage metalloelastase



### 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: Macrophage metalloelastase



## 5 Refinement protocol and experimental data overview

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

Of the 14 calculated structures, 14 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
GROMACS	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)	2mlr_cs.str
Number of chemical shift lists	1
Total number of shifts	1762
Number of shifts mapped to atoms	1762
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

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: ZN, CA, 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	0.58±0.01	0±0/1305 (0.0±0.0%)	2.04±0.06	42±6/1768 (2.4±0.4%)
All	All	0.58	0/18270 (0.0%)	2.05	584/24752 (2.4%)

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	5.1±1.9
All	All	0	71

There are no bond-length outliers.

5 of 249 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	249	ARG	NE-CZ-NH1	19.17	129.88	120.30	11	6
1	A	127	ARG	NE-CZ-NH2	-18.79	110.91	120.30	11	8
1	A	165	ARG	NE-CZ-NH2	-18.12	111.24	120.30	5	4
1	A	262	TYR	CB-CG-CD2	-17.25	110.65	121.00	14	4
1	A	240	TYR	CB-CG-CD1	-14.90	112.06	121.00	6	5

There are no chirality outliers.

5 of 36 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	242	TYR	Peptide,Sidechain	7

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	204	THR	Peptide	5
1	A	262	TYR	Sidechain	5
1	A	121	TYR	Sidechain	5
1	A	240	TYR	Sidechain,Peptide	4

## 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	1265	1199	1196	2±1
4	A	5750	0	9000	131±13
All	All	98280	16786	142744	1846

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 8.

5 of 1763 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
4:A:388:PX4:H39	4:A:411:PX4:H17	0.99	1.35	4	1
4:A:337:PX4:H47	4:A:353:PX4:H15	0.93	1.41	8	2
4:A:413:PX4:H24	4:A:430:PX4:H63	0.92	1.40	10	1
4:A:320:PX4:H20	4:A:359:PX4:H57	0.92	1.42	5	1
4:A:368:PX4:H22	4:A:369:PX4:H51	0.90	1.40	6	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	158/164 (96%)	145±3 (92±2%)	12±3 (8±2%)	1±1 (1±0%)	34	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2212/2296 (96%)	2030 (92%)	168 (8%)	14 (1%)	34	78

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	171	PHE	5
1	A	175	ASP	3
1	A	107	PRO	2
1	A	213	PHE	1
1	A	179	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	129/131 (98%)	123±2 (95±2%)	6±2 (5±2%)	35	79
All	All	1806/1834 (98%)	1716 (95%)	90 (5%)	35	79

5 of 25 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	244	ASP	14
1	A	101	ARG	14
1	A	199	GLU	9
1	A	222	HIS	8
1	A	249	ARG	7

### 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 130 ligands modelled in this entry, 5 are monoatomic - leaving 125 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	306	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	307	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	308	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	309	-	45,45,45	0.66±0.02	0±0 (0±0%)
4	PX4	A	310	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	311	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	312	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	313	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	314	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	315	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	316	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	317	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	318	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	319	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	320	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	321	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	322	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	323	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	324	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	325	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	326	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	327	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	328	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	329	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	330	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	331	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	332	-	45,45,45	0.65±0.02	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	333	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	334	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	335	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	336	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	337	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	338	-	45,45,45	0.66±0.01	0±0 (0±0%)
4	PX4	A	339	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	340	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	341	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	342	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	343	-	45,45,45	0.66±0.01	0±0 (0±0%)
4	PX4	A	344	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	345	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	346	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	347	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	348	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	349	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	350	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	351	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	352	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	353	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	354	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	355	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	356	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	357	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	358	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	359	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	360	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	361	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	362	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	363	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	364	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	365	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	366	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	367	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	368	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	369	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	370	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	371	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	372	-	45,45,45	0.66±0.02	0±0 (0±0%)
4	PX4	A	373	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	374	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	375	-	45,45,45	0.65±0.01	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	376	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	377	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	378	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	379	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	380	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	381	-	45,45,45	0.64±0.03	0±0 (0±0%)
4	PX4	A	382	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	383	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	384	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	385	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	386	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	387	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	388	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	389	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	390	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	391	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	392	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	393	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	394	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	395	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	396	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	397	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	398	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	399	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	400	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	401	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	402	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	403	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	404	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	405	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	406	-	45,45,45	0.66±0.02	0±0 (0±0%)
4	PX4	A	407	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	408	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	409	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	410	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	411	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	412	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	413	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	414	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	415	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	416	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	417	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	418	-	45,45,45	0.64±0.02	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
4	PX4	A	419	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	420	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	421	-	45,45,45	0.64±0.02	0±0 (0±0%)
4	PX4	A	422	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	423	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	424	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	425	-	45,45,45	0.65±0.01	0±0 (0±0%)
4	PX4	A	426	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	427	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	428	-	45,45,45	0.65±0.02	0±0 (0±0%)
4	PX4	A	429	-	45,45,45	0.64±0.01	0±0 (0±0%)
4	PX4	A	430	-	45,45,45	0.65±0.01	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	PX4	A	306	-	49,53,53	1.47±0.07	0±0 (0±0%)
4	PX4	A	307	-	49,53,53	1.55±0.19	0±0 (0±0%)
4	PX4	A	308	-	49,53,53	1.48±0.15	0±0 (0±0%)
4	PX4	A	309	-	49,53,53	1.47±0.15	0±0 (0±0%)
4	PX4	A	310	-	49,53,53	1.44±0.16	0±0 (0±0%)
4	PX4	A	311	-	49,53,53	1.52±0.20	0±1 (0±1%)
4	PX4	A	312	-	49,53,53	1.45±0.18	0±1 (0±1%)
4	PX4	A	313	-	49,53,53	1.48±0.15	0±0 (0±0%)
4	PX4	A	314	-	49,53,53	1.46±0.16	0±0 (0±0%)
4	PX4	A	315	-	49,53,53	1.40±0.13	0±0 (0±0%)
4	PX4	A	316	-	49,53,53	1.41±0.11	0±0 (0±0%)
4	PX4	A	317	-	49,53,53	1.41±0.14	0±0 (0±0%)
4	PX4	A	318	-	49,53,53	1.42±0.15	0±0 (0±0%)
4	PX4	A	319	-	49,53,53	1.48±0.15	0±0 (0±0%)
4	PX4	A	320	-	49,53,53	1.44±0.16	0±1 (0±1%)
4	PX4	A	321	-	49,53,53	1.42±0.14	0±0 (0±0%)
4	PX4	A	322	-	49,53,53	1.48±0.17	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	323	-	49,53,53	1.39±0.17	0±0 (0±0%)
4	PX4	A	324	-	49,53,53	1.41±0.16	0±0 (0±0%)
4	PX4	A	325	-	49,53,53	1.47±0.14	0±0 (0±0%)
4	PX4	A	326	-	49,53,53	1.42±0.19	0±0 (0±0%)
4	PX4	A	327	-	49,53,53	1.53±0.12	0±0 (0±1%)
4	PX4	A	328	-	49,53,53	1.47±0.14	0±0 (0±0%)
4	PX4	A	329	-	49,53,53	1.48±0.12	0±0 (0±0%)
4	PX4	A	330	-	49,53,53	1.44±0.13	0±0 (0±0%)
4	PX4	A	331	-	49,53,53	1.49±0.13	0±0 (0±0%)
4	PX4	A	332	-	49,53,53	1.44±0.14	0±0 (0±0%)
4	PX4	A	333	-	49,53,53	1.48±0.16	0±0 (0±0%)
4	PX4	A	334	-	49,53,53	1.49±0.12	0±0 (0±0%)
4	PX4	A	335	-	49,53,53	1.45±0.14	0±0 (0±0%)
4	PX4	A	336	-	49,53,53	1.46±0.19	0±0 (0±0%)
4	PX4	A	337	-	49,53,53	1.42±0.19	0±0 (0±0%)
4	PX4	A	338	-	49,53,53	1.50±0.16	0±0 (0±0%)
4	PX4	A	339	-	49,53,53	1.42±0.23	0±1 (0±1%)
4	PX4	A	340	-	49,53,53	1.53±0.10	0±0 (0±0%)
4	PX4	A	341	-	49,53,53	1.46±0.14	0±0 (0±0%)
4	PX4	A	342	-	49,53,53	1.48±0.14	0±0 (0±0%)
4	PX4	A	343	-	49,53,53	1.43±0.19	0±0 (0±0%)
4	PX4	A	344	-	49,53,53	1.49±0.16	0±0 (0±0%)
4	PX4	A	345	-	49,53,53	1.41±0.17	0±0 (0±0%)
4	PX4	A	346	-	49,53,53	1.44±0.15	0±0 (0±0%)
4	PX4	A	347	-	49,53,53	1.45±0.20	0±0 (0±0%)
4	PX4	A	348	-	49,53,53	1.46±0.16	0±1 (0±1%)
4	PX4	A	349	-	49,53,53	1.49±0.12	0±0 (0±0%)
4	PX4	A	350	-	49,53,53	1.40±0.11	0±0 (0±0%)
4	PX4	A	351	-	49,53,53	1.47±0.14	0±0 (0±0%)
4	PX4	A	352	-	49,53,53	1.47±0.14	0±0 (0±0%)
4	PX4	A	353	-	49,53,53	1.47±0.11	0±0 (0±1%)
4	PX4	A	354	-	49,53,53	1.53±0.15	0±0 (0±0%)
4	PX4	A	355	-	49,53,53	1.44±0.13	0±0 (0±0%)
4	PX4	A	356	-	49,53,53	1.48±0.19	0±0 (0±0%)
4	PX4	A	357	-	49,53,53	1.45±0.13	0±0 (0±0%)
4	PX4	A	358	-	49,53,53	1.42±0.14	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	359	-	49,53,53	1.50±0.15	0±1 (0±1%)
4	PX4	A	360	-	49,53,53	1.47±0.12	0±1 (0±1%)
4	PX4	A	361	-	49,53,53	1.50±0.12	0±0 (0±0%)
4	PX4	A	362	-	49,53,53	1.47±0.07	0±0 (0±0%)
4	PX4	A	363	-	49,53,53	1.42±0.16	0±0 (0±0%)
4	PX4	A	364	-	49,53,53	1.51±0.20	0±0 (0±0%)
4	PX4	A	365	-	49,53,53	1.46±0.13	0±0 (0±0%)
4	PX4	A	366	-	49,53,53	1.48±0.12	0±0 (0±0%)
4	PX4	A	367	-	49,53,53	1.46±0.17	0±0 (0±0%)
4	PX4	A	368	-	49,53,53	1.47±0.14	0±0 (0±0%)
4	PX4	A	369	-	49,53,53	1.36±0.14	0±0 (0±0%)
4	PX4	A	370	-	49,53,53	1.45±0.12	0±0 (0±0%)
4	PX4	A	371	-	49,53,53	1.65±0.16	0±0 (0±0%)
4	PX4	A	372	-	49,53,53	1.43±0.16	0±0 (0±0%)
4	PX4	A	373	-	49,53,53	1.56±0.16	0±0 (0±0%)
4	PX4	A	374	-	49,53,53	1.43±0.15	0±0 (0±0%)
4	PX4	A	375	-	49,53,53	1.48±0.16	0±0 (0±0%)
4	PX4	A	376	-	49,53,53	1.47±0.18	0±0 (0±0%)
4	PX4	A	377	-	49,53,53	1.50±0.19	0±1 (0±1%)
4	PX4	A	378	-	49,53,53	1.41±0.16	0±0 (0±0%)
4	PX4	A	379	-	49,53,53	1.50±0.13	0±0 (0±0%)
4	PX4	A	380	-	49,53,53	1.44±0.16	0±1 (0±1%)
4	PX4	A	381	-	49,53,53	1.54±0.14	0±1 (0±1%)
4	PX4	A	382	-	49,53,53	1.42±0.16	0±0 (0±0%)
4	PX4	A	383	-	49,53,53	1.40±0.11	0±0 (0±0%)
4	PX4	A	384	-	49,53,53	1.46±0.22	0±0 (0±0%)
4	PX4	A	385	-	49,53,53	1.49±0.17	0±0 (0±0%)
4	PX4	A	386	-	49,53,53	1.44±0.16	0±0 (0±0%)
4	PX4	A	387	-	49,53,53	1.50±0.16	0±0 (0±0%)
4	PX4	A	388	-	49,53,53	1.41±0.14	0±0 (0±0%)
4	PX4	A	389	-	49,53,53	1.50±0.16	0±0 (0±0%)
4	PX4	A	390	-	49,53,53	1.44±0.13	0±0 (0±0%)
4	PX4	A	391	-	49,53,53	1.48±0.15	0±0 (0±0%)
4	PX4	A	392	-	49,53,53	1.51±0.13	0±0 (0±0%)
4	PX4	A	393	-	49,53,53	1.52±0.13	0±0 (0±0%)
4	PX4	A	394	-	49,53,53	1.48±0.15	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	395	-	49,53,53	1.47±0.13	0±0 (0±0%)
4	PX4	A	396	-	49,53,53	1.51±0.18	1±1 (1±1%)
4	PX4	A	397	-	49,53,53	1.49±0.19	0±0 (0±0%)
4	PX4	A	398	-	49,53,53	1.44±0.16	0±0 (0±0%)
4	PX4	A	399	-	49,53,53	1.44±0.16	0±0 (0±0%)
4	PX4	A	400	-	49,53,53	1.46±0.19	0±1 (0±1%)
4	PX4	A	401	-	49,53,53	1.54±0.15	0±1 (0±1%)
4	PX4	A	402	-	49,53,53	1.40±0.15	0±0 (0±0%)
4	PX4	A	403	-	49,53,53	1.47±0.14	0±0 (0±0%)
4	PX4	A	404	-	49,53,53	1.51±0.16	0±0 (0±0%)
4	PX4	A	405	-	49,53,53	1.45±0.14	0±0 (0±0%)
4	PX4	A	406	-	49,53,53	1.42±0.14	0±0 (0±0%)
4	PX4	A	407	-	49,53,53	1.42±0.18	0±0 (0±0%)
4	PX4	A	408	-	49,53,53	1.47±0.15	0±0 (0±0%)
4	PX4	A	409	-	49,53,53	1.48±0.10	0±0 (0±0%)
4	PX4	A	410	-	49,53,53	1.46±0.18	0±0 (0±0%)
4	PX4	A	411	-	49,53,53	1.44±0.11	0±0 (0±0%)
4	PX4	A	412	-	49,53,53	1.39±0.13	0±0 (0±0%)
4	PX4	A	413	-	49,53,53	1.47±0.13	0±0 (0±0%)
4	PX4	A	414	-	49,53,53	1.50±0.14	0±0 (0±0%)
4	PX4	A	415	-	49,53,53	1.53±0.17	0±1 (0±1%)
4	PX4	A	416	-	49,53,53	1.44±0.17	0±0 (0±0%)
4	PX4	A	417	-	49,53,53	1.51±0.16	0±0 (0±0%)
4	PX4	A	418	-	49,53,53	1.45±0.15	0±0 (0±0%)
4	PX4	A	419	-	49,53,53	1.48±0.12	0±0 (0±0%)
4	PX4	A	420	-	49,53,53	1.46±0.13	0±0 (0±0%)
4	PX4	A	421	-	49,53,53	1.45±0.13	0±1 (0±1%)
4	PX4	A	422	-	49,53,53	1.48±0.13	0±0 (0±0%)
4	PX4	A	423	-	49,53,53	1.44±0.12	0±0 (0±0%)
4	PX4	A	424	-	49,53,53	1.39±0.18	0±0 (0±0%)
4	PX4	A	425	-	49,53,53	1.42±0.11	0±0 (0±0%)
4	PX4	A	426	-	49,53,53	1.43±0.14	0±1 (0±1%)
4	PX4	A	427	-	49,53,53	1.59±0.18	0±0 (0±0%)
4	PX4	A	428	-	49,53,53	1.50±0.10	0±0 (0±0%)
4	PX4	A	429	-	49,53,53	1.45±0.18	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
4	PX4	A	430	-	49,53,53	1.55±0.14	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PX4	A	306	-	-	0±0,49,49,49	0±0,0,0,0
4	PX4	A	307	-	-	2±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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	-	0±0,49,49,49	0±0,0,0,0
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	-	-	2±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	-	-	0±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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

There are no bond-length outliers.

5 of 199 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	417	PX4	O7-C23-C24	7.71	127.78	111.53	6	2
4	A	413	PX4	C8-C7-C6	7.21	95.29	112.08	8	1
4	A	396	PX4	C8-C7-C6	7.14	95.44	112.08	3	6
4	A	426	PX4	O7-C23-C24	7.00	126.28	111.53	7	1
4	A	385	PX4	O7-C23-C24	6.99	126.27	111.53	6	1

There are no chirality outliers.

All 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	371	PX4	C7-O7-C23-O8	14
4	A	371	PX4	C7-O7-C23-C24	14
4	A	307	PX4	C7-O7-C23-C24	12
4	A	307	PX4	C7-O7-C23-O8	11

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

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 83% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2mlr\_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	1762
Number of shifts mapped to atoms	1762
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	160	$-0.25 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	138	$0.11 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	129	$-0.17 \pm 0.15$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	154	$-0.70 \pm 0.49$	None needed (imprecise)

#### 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 83%, i.e. 1600 atoms were assigned a chemical shift out of a possible 1936. 15 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	740/786 (94%)	306/313 (98%)	284/320 (89%)	150/153 (98%)
Sidechain	712/887 (80%)	443/521 (85%)	260/326 (80%)	9/40 (22%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	148/263 (56%)	79/142 (56%)	66/109 (61%)	3/12 (25%)
Overall	1600/1936 (83%)	828/976 (85%)	610/755 (81%)	162/205 (79%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	226	LEU	CG	33.00	32.55 – 21.05	5.4
1	A	214	LEU	CG	33.00	32.55 – 21.05	5.4

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

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:

