



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2018 – 04:00 PM EST

PDB ID : 4D65  
Title : Structure of porin Omp-Pst2 from *P. stuartii*; the asymmetric unit contains a dimer of trimers.  
Authors : Nasrallah, C.; Colletier, J.P.  
Deposited on : 2014-11-08  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

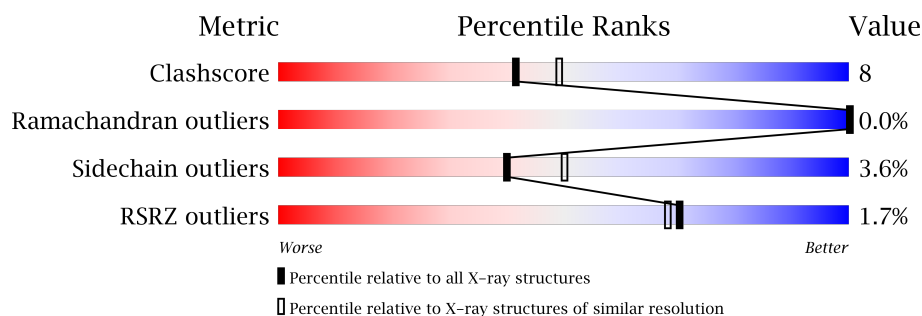
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	343	<div> <div>0.0%</div> <div>86%</div> <div>13%</div> <div>0.0%</div> </div>
1	B	343	<div> <div>0.0%</div> <div>92%</div> <div>8%</div> <div>0.0%</div> </div>
1	C	343	<div> <div>3%</div> <div>88%</div> <div>10%</div> <div>0.0%</div> </div>
1	D	343	<div> <div>2%</div> <div>92%</div> <div>7%</div> <div>0.0%</div> </div>
1	E	343	<div> <div>2%</div> <div>92%</div> <div>8%</div> <div>0.0%</div> </div>
1	F	343	<div> <div>0.0%</div> <div>92%</div> <div>8%</div> <div>0.0%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LDA	A	1344	-	-	-	X
2	LDA	A	1345	-	-	-	X
2	LDA	A	1346	-	-	-	X
2	LDA	A	1348	-	-	-	X
2	LDA	A	1350[B]	-	-	X	-
2	LDA	A	1352	-	-	-	X
2	LDA	A	1353	-	-	-	X
2	LDA	A	1354	-	-	X	X
2	LDA	A	1357	-	-	-	X
2	LDA	A	1359	-	-	-	X
2	LDA	A	1360	-	-	-	X
2	LDA	A	1361	-	-	-	X
2	LDA	A	1362	-	-	-	X
2	LDA	A	1364	-	-	-	X
2	LDA	A	1365	-	-	-	X
2	LDA	A	1366	-	-	-	X
2	LDA	A	1369	-	-	-	X
2	LDA	A	1370	-	-	-	X
2	LDA	A	1371	-	-	-	X
2	LDA	A	1372	-	-	-	X
2	LDA	A	1373	-	-	-	X
2	LDA	A	1376	-	-	-	X
2	LDA	A	1379	-	-	-	X
2	LDA	A	1383	-	-	-	X
2	LDA	A	1387	-	-	X	X
2	LDA	A	1500	-	-	-	X
2	LDA	A	1501	-	-	-	X
2	LDA	B	1344	-	-	-	X
2	LDA	B	1345	-	-	-	X
2	LDA	B	1347	-	-	-	X
2	LDA	B	1348	-	-	-	X
2	LDA	B	1350	-	-	-	X
2	LDA	B	1352	-	-	-	X
2	LDA	B	1353	-	-	-	X
2	LDA	B	1354	-	-	-	X
2	LDA	B	1358	-	-	-	X
2	LDA	B	1359	-	-	-	X
2	LDA	B	1360	-	-	-	X
2	LDA	B	1363	-	-	-	X
2	LDA	B	1364	-	-	-	X
2	LDA	B	1365	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LDA	B	1500	-	-	-	X
2	LDA	B	1501	-	-	-	X
2	LDA	C	1344	-	-	-	X
2	LDA	C	1345	-	-	-	X
2	LDA	C	1346	-	-	-	X
2	LDA	C	1348	-	-	-	X
2	LDA	C	1351	-	-	-	X
2	LDA	C	1353	-	-	-	X
2	LDA	C	1356	-	-	-	X
2	LDA	C	1357	-	-	-	X
2	LDA	C	1358	-	-	-	X
2	LDA	C	1362	-	-	-	X
2	LDA	D	1344	-	-	-	X
2	LDA	D	1345	-	-	-	X
2	LDA	D	1347	-	-	-	X
2	LDA	D	1348	-	-	-	X
2	LDA	D	1350	-	-	-	X
2	LDA	D	1352	-	-	-	X
2	LDA	D	1353	-	-	-	X
2	LDA	D	1361	-	-	-	X
2	LDA	E	1344	-	-	-	X
2	LDA	E	1345	-	-	-	X
2	LDA	E	1348	-	-	-	X
2	LDA	E	1349	-	-	-	X
2	LDA	E	1352	-	-	-	X
2	LDA	E	1353	-	-	-	X
2	LDA	E	1356	-	-	-	X
2	LDA	E	1357	-	-	-	X
2	LDA	F	1344	-	-	-	X
2	LDA	F	1345	-	-	-	X
2	LDA	F	1346	-	-	-	X
2	LDA	F	1347	-	-	-	X
2	LDA	F	1348	-	-	-	X
2	LDA	F	1349	-	-	-	X
2	LDA	F	1350	-	-	-	X
2	LDA	F	1351	-	-	-	X
2	LDA	F	1352	-	-	-	X
2	LDA	F	1353	-	-	-	X
2	LDA	F	1354	-	-	-	X
2	LDA	F	1355	-	-	-	X
2	LDA	F	1357	-	-	-	X
2	LDA	F	1359	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LDA	F	1361	-	-	-	X
2	LDA	F	1365	-	-	-	X
3	FTT	B	1375	-	-	-	X
3	FTT	C	1363	-	-	-	X
3	FTT	D	1364	X	-	-	X
4	MYR	B	1376	-	-	-	X
4	MYR	C	1364	-	-	-	X
4	MYR	C	1366	-	-	-	X

## 2 Entry composition [i](#)

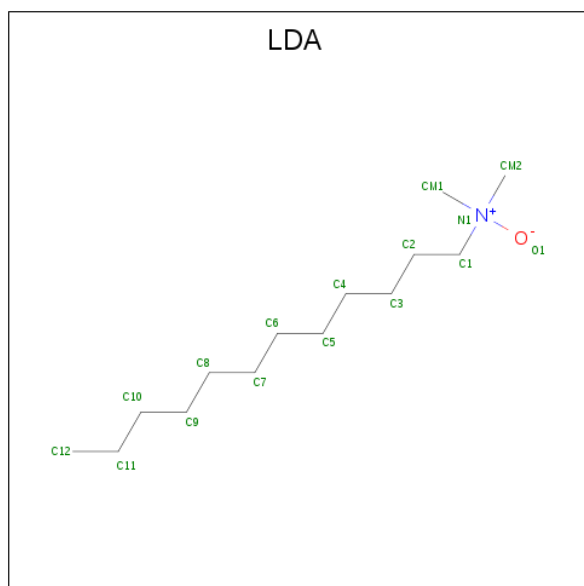
There are 6 unique types of molecules in this entry. The entry contains 22075 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PORIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	4	0
			2711	1691	459	556	5			
1	B	343	Total	C	N	O	S	0	8	0
			2749	1719	464	561	5			
1	C	343	Total	C	N	O	S	0	8	0
			2745	1715	465	560	5			
1	D	343	Total	C	N	O	S	0	5	0
			2717	1694	460	558	5			
1	E	343	Total	C	N	O	S	0	8	0
			2749	1718	466	560	5			
1	F	343	Total	C	N	O	S	0	3	0
			2706	1689	458	554	5			

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	1
			32	28	2	2		
2	A	1	Total	C	N	O	0	0
			14	12	1	1		
2	A	1	Total	C	N	O	0	0
			12	10	1	1		
2	A	1	Total	C	N	O	0	0
			11	9	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			11	9	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C			0	0
			8	8				
2	A	1	Total	C	N	O	0	0
			12	10	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C			0	0
			9	9				
2	A	1	Total	C			0	0
			9	9				
2	A	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C			0	0
			8	8				
2	A	1	Total	C			0	0
			9	9				
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C			0	0
			9	9				
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			11	9	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C			0	0
			11	11				
2	A	1	Total	C	N	O	0	0
			11	9	1	1		
2	A	1	Total	C	N	O	0	0
			11	9	1	1		
2	B	1	Total	C	N	O	0	0
			10	8	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			13	11	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C			0	0
			9	9				
2	B	1	Total	C	N	O	0	0
			12	10	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C			0	0
			9	9				
2	B	1	Total	C			0	0
			9	9				
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			11	9	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			8	6	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			11	9	1	1		
2	C	1	Total	C	N	O	0	0
			8	6	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			11	9	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			11	9	1	1		
2	C	1	Total	C	N	O	0	0
			9	7	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C			0	0
			10	10				
2	C	1	Total	C	N	O	0	0
			11	9	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			11	9	1	1		
2	C	1	Total	C			0	0
			8	8				
2	D	1	Total	C	N	O	0	0
			16	14	1	1		
2	D	1	Total	C	N	O	0	0
			16	14	1	1		
2	D	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			16	14	1	1		
2	D	1	Total	C	N	O	0	0
			16	14	1	1		
2	D	1	Total	C	N	O	0	0
			16	14	1	1		
2	D	1	Total	C	N	O	0	0
			11	9	1	1		
2	D	1	Total	C	N	O	0	0
			11	9	1	1		
2	D	1	Total	C	N	O	0	0
			16	14	1	1		
2	D	1	Total	C	N	O	0	0
			16	14	1	1		
2	D	1	Total	C	N	O	0	0
			14	12	1	1		
2	D	1	Total	C	N	O	0	0
			16	14	1	1		
2	D	1	Total	C	N	O	0	0
			16	14	1	1		
2	D	1	Total	C	N	O	0	0
			16	14	1	1		
2	D	1	Total	C			0	0
			8	8				
2	D	1	Total	C			0	0
			8	8				
2	D	1	Total	C	N	O	0	0
			16	14	1	1		
2	D	1	Total	C			0	0
			8	8				
2	D	1	Total	C	N	O	0	0
			16	14	1	1		
2	D	1	Total	C	N	O	0	0
			16	14	1	1		
2	E	1	Total	C	N	O	0	0
			16	14	1	1		
2	E	1	Total	C	N	O	0	0
			11	9	1	1		
2	E	1	Total	C	N	O	0	0
			11	9	1	1		
2	E	1	Total	C	N	O	0	0
			11	9	1	1		

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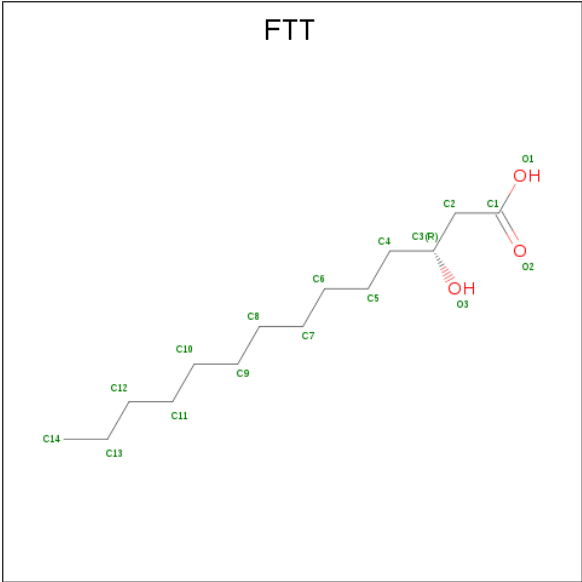
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2	E	1	Total 14	C 12	N 1	O 1	0	0
2	E	1	Total 16	C 14	N 1	O 1	0	0
2	E	1	Total 11	C 9	N 1	O 1	0	0
2	E	1	Total 16	C 14	N 1	O 1	0	0
2	E	1	Total 10	C 10			0	0
2	E	1	Total 16	C 14	N 1	O 1	0	0
2	E	1	Total 16	C 14	N 1	O 1	0	0
2	E	1	Total 16	C 14	N 1	O 1	0	0
2	E	1	Total 16	C 14	N 1	O 1	0	0
2	F	1	Total 16	C 14	N 1	O 1	0	0
2	F	1	Total 16	C 14	N 1	O 1	0	0
2	F	1	Total 16	C 14	N 1	O 1	0	0
2	F	1	Total 16	C 14	N 1	O 1	0	0
2	F	1	Total 16	C 14	N 1	O 1	0	0
2	F	1	Total 16	C 14	N 1	O 1	0	0
2	F	1	Total 16	C 14	N 1	O 1	0	0
2	F	1	Total 16	C 14	N 1	O 1	0	0
2	F	1	Total 16	C 14	N 1	O 1	0	0
2	F	1	Total 16	C 14	N 1	O 1	0	0
2	F	1	Total 16	C 14	N 1	O 1	0	0

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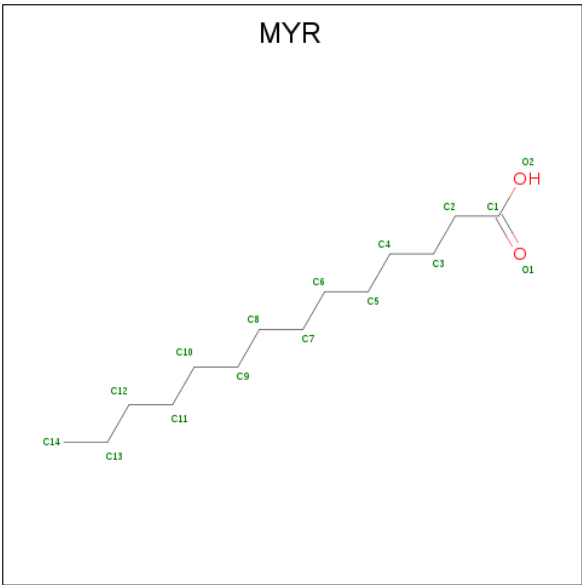
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total	C	N	O	0	0
			11	9	1	1		
2	F	1	Total	C	N	O	0	0
			11	9	1	1		
2	F	1	Total	C	N	O	0	0
			16	14	1	1		
2	F	1	Total	C	N	O	0	0
			16	14	1	1		
2	F	1	Total	C	N	O	0	0
			16	14	1	1		
2	F	1	Total	C	N	O	0	0
			16	14	1	1		
2	F	1	Total	C	N	O	0	0
			16	14	1	1		
2	F	1	Total	C	N	O	0	0
			16	14	1	1		
2	F	1	Total	C	N	O	0	0
			16	14	1	1		
2	F	1	Total	C	N	O	0	0
			16	14	1	1		
2	F	1	Total	C	N	O	0	0
			16	14	1	1		
2	F	1	Total	C	N	O	0	0
			12	10	1	1		
2	F	1	Total	C	N	O	0	0
			16	14	1	1		
2	F	1	Total	C			0	0
			10	10				
2	F	1	Total	C	N	O	0	0
			16	14	1	1		
2	F	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 3 is 3-HYDROXY-TETRADECANOIC ACID (three-letter code: FTT) (formula:  $C_{14}H_{28}O_3$ ).



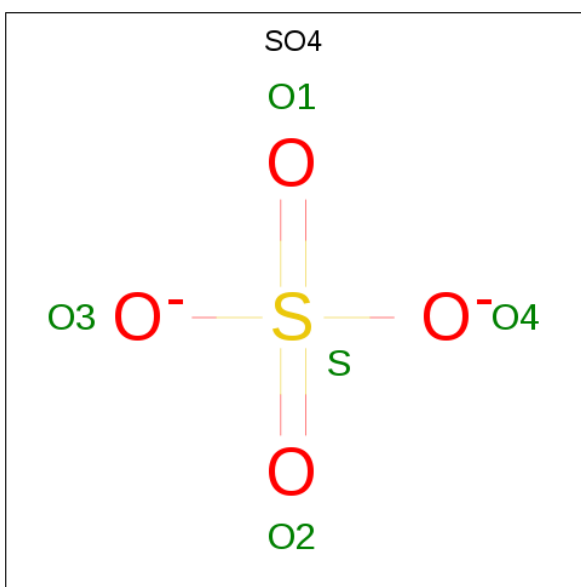
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			16	14	2		
3	C	1	Total	C	O	0	0
			16	14	2		
3	C	1	Total	C	O	0	0
			16	14	2		
3	C	1	Total	C	O	0	0
			16	14	2		
3	C	1	Total	C	O	0	0
			16	14	2		
3	D	1	Total	C	O	0	0
			16	14	2		

- Molecule 4 is MYRISTIC ACID (three-letter code: MYR) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			15	14	1		
4	C	1	Total	C	O	0	0
			15	14	1		
4	C	1	Total	C	O	0	0
			15	14	1		
4	C	1	Total	C	O	0	0
			15	14	1		
4	C	1	Total	C	O	0	0
			15	14	1		
4	D	1	Total	C	O	0	0
			15	14	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

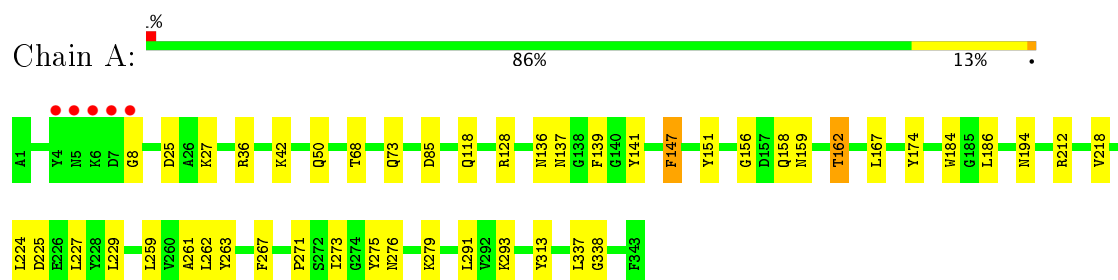
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	592	Total	O	0	0
			592	592		
6	B	547	Total	O	0	0
			547	547		
6	C	502	Total	O	0	0
			502	502		
6	D	584	Total	O	0	0
			584	584		
6	E	491	Total	O	0	0
			491	491		
6	F	399	Total	O	0	0
			399	399		

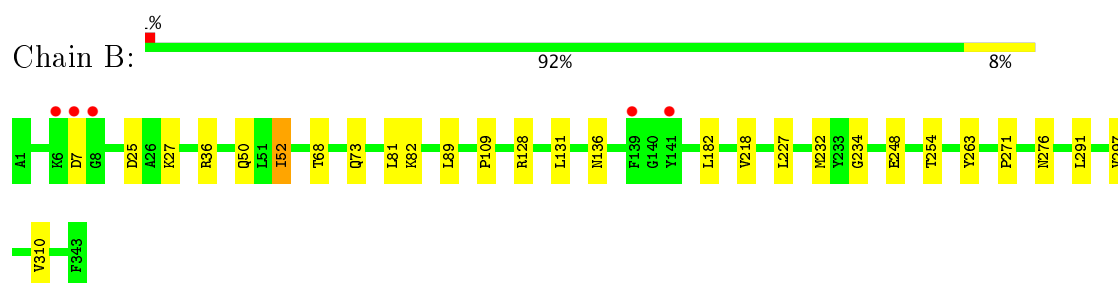
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

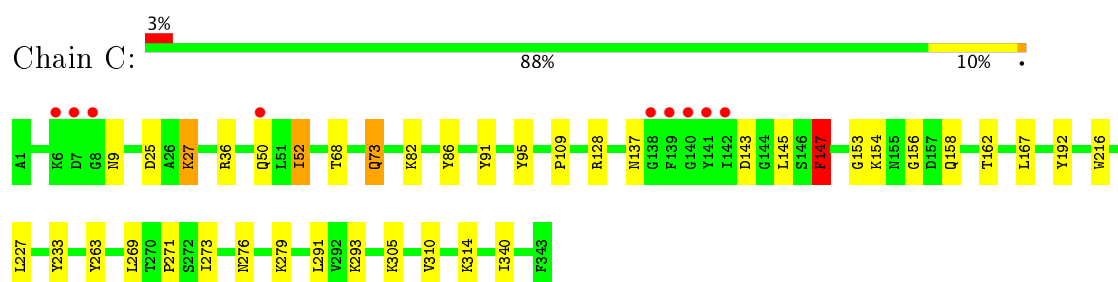
#### • Molecule 1: PORIN 2



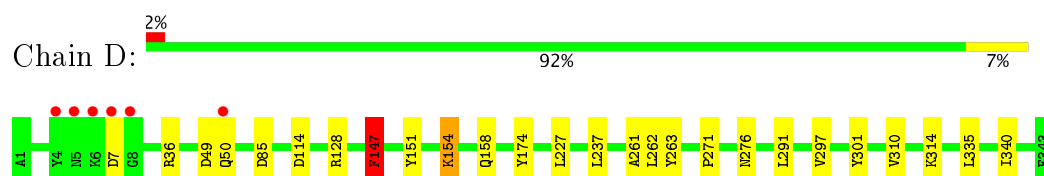
#### • Molecule 1: PORIN 2



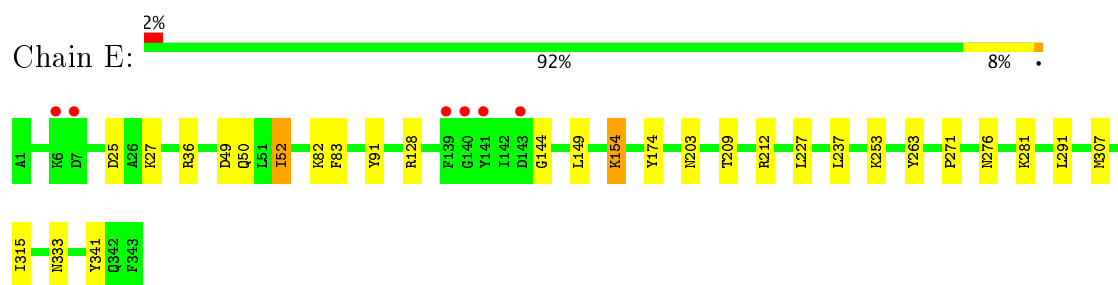
#### • Molecule 1: PORIN 2



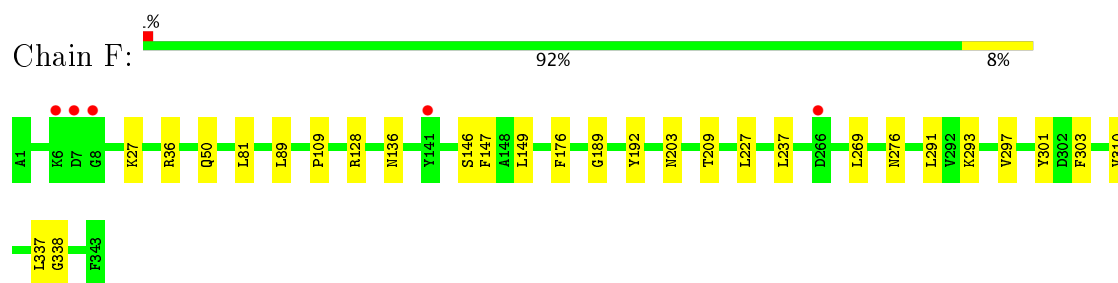
#### • Molecule 1: PORIN 2



#### • Molecule 1: PORIN 2



• Molecule 1: PORIN 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.26Å 135.51Å 151.71Å 90.00° 114.61° 90.00°	Depositor
Resolution (Å)	45.72 – 2.20 46.49 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.5 (45.72-2.20) 93.5 (46.49-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.167 , 0.197 0.160 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	35.3	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 76.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	22075	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, MYR, FTT, SO4

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 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	1.57	6/2769 (0.2%)	1.37	10/3742 (0.3%)
1	B	0.35	0/2803	0.52	0/3788
1	C	3.28	7/2803 (0.2%)	2.77	14/3786 (0.4%)
1	D	3.51	6/2775 (0.2%)	2.29	8/3750 (0.2%)
1	E	0.35	0/2801	0.54	0/3782
1	F	0.35	0/2758	0.53	0/3726
All	All	2.08	19/16709 (0.1%)	1.62	32/22574 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	147[A]	PHE	CD1-CE1	118.71	3.76	1.39
1	C	147[B]	PHE	CD1-CE1	118.71	3.76	1.39
1	D	147[A]	PHE	CD1-CE1	110.84	3.60	1.39
1	D	147[B]	PHE	CD1-CE1	110.84	3.60	1.39
1	D	147[A]	PHE	CG-CD1	67.57	2.40	1.38
1	D	147[B]	PHE	CG-CD1	67.57	2.40	1.38
1	A	147[A]	PHE	CD1-CE1	45.87	2.31	1.39
1	A	147[B]	PHE	CD1-CE1	45.87	2.31	1.39
1	A	147[A]	PHE	CG-CD1	28.90	1.82	1.38
1	A	147[B]	PHE	CG-CD1	28.90	1.82	1.38
1	C	147[A]	PHE	CG-CD1	25.39	1.76	1.38
1	C	147[B]	PHE	CG-CD1	25.39	1.76	1.38
1	A	147[A]	PHE	CB-CG	-16.87	1.22	1.51
1	A	147[B]	PHE	CB-CG	-16.87	1.22	1.51
1	C	147[A]	PHE	CB-CG	-12.00	1.30	1.51
1	C	147[B]	PHE	CB-CG	-12.00	1.30	1.51
1	C	153	GLY	C-N	-11.16	1.08	1.34
1	D	147[A]	PHE	CB-CG	-5.69	1.41	1.51
1	D	147[B]	PHE	CB-CG	-5.69	1.41	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	147[A]	PHE	CG-CD1-CE1	-82.54	30.00	120.80
1	C	147[B]	PHE	CG-CD1-CE1	-82.54	30.00	120.80
1	D	147[A]	PHE	CG-CD1-CE1	-72.06	41.53	120.80
1	D	147[B]	PHE	CG-CD1-CE1	-72.06	41.53	120.80
1	D	147[A]	PHE	CB-CG-CD1	-63.44	76.39	120.80
1	D	147[B]	PHE	CB-CG-CD1	-63.44	76.39	120.80
1	C	147[A]	PHE	CD1-CG-CD2	-60.92	39.10	118.30
1	C	147[B]	PHE	CD1-CG-CD2	-60.92	39.10	118.30
1	A	147[A]	PHE	CG-CD1-CE1	-45.82	70.40	120.80
1	A	147[B]	PHE	CG-CD1-CE1	-45.82	70.40	120.80
1	C	147[A]	PHE	CD1-CE1-CZ	-43.27	68.18	120.10
1	C	147[B]	PHE	CD1-CE1-CZ	-43.27	68.18	120.10
1	C	147[A]	PHE	CB-CG-CD2	32.56	143.59	120.80
1	C	147[B]	PHE	CB-CG-CD2	32.56	143.59	120.80
1	C	147[A]	PHE	CB-CG-CD1	-19.50	107.15	120.80
1	C	147[B]	PHE	CB-CG-CD1	-19.50	107.15	120.80
1	A	147[A]	PHE	CB-CG-CD1	-18.39	107.93	120.80
1	A	147[B]	PHE	CB-CG-CD1	-18.39	107.93	120.80
1	A	147[A]	PHE	CA-CB-CG	15.68	151.54	113.90
1	A	147[B]	PHE	CA-CB-CG	15.68	151.54	113.90
1	A	147[A]	PHE	CD1-CG-CD2	13.71	136.12	118.30
1	A	147[B]	PHE	CD1-CG-CD2	13.71	136.12	118.30
1	A	147[A]	PHE	CB-CG-CD2	-11.25	112.92	120.80
1	A	147[B]	PHE	CB-CG-CD2	-11.25	112.92	120.80
1	C	147[A]	PHE	CA-CB-CG	10.74	139.68	113.90
1	C	147[B]	PHE	CA-CB-CG	10.74	139.68	113.90
1	C	153	GLY	C-N-CA	7.80	141.20	121.70
1	C	153	GLY	O-C-N	-6.81	111.80	122.70
1	D	147[A]	PHE	CD1-CE1-CZ	-6.64	112.13	120.10
1	D	147[B]	PHE	CD1-CE1-CZ	-6.64	112.13	120.10
1	D	147[A]	PHE	CA-CB-CG	5.13	126.21	113.90
1	D	147[B]	PHE	CA-CB-CG	5.13	126.21	113.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2711	0	2528	41	0
1	B	2749	0	2570	19	0
1	C	2745	0	2571	27	0
1	D	2717	0	2532	20	0
1	E	2749	0	2582	20	0
1	F	2706	0	2531	16	0
2	A	700	0	1306	77	0
2	B	481	0	905	39	0
2	C	298	0	547	26	0
2	D	284	0	530	27	0
2	E	196	0	360	17	0
2	F	428	0	816	53	0
3	B	16	0	26	0	0
3	C	64	0	104	8	0
3	D	16	0	26	0	0
4	B	15	0	27	0	0
4	C	60	0	108	6	0
4	D	15	0	27	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	A	592	0	0	12	0
6	B	547	0	0	6	0
6	C	502	0	0	10	0
6	D	584	0	0	7	0
6	E	491	0	0	3	0
6	F	399	0	0	5	0
All	All	22075	0	20096	314	0

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.

All (314) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147[A]:PHE:HB3	1:D:147[A]:PHE:CD1	1.79	1.16
2:A:1357:LDA:HM12	2:A:1373:LDA:HM22	1.33	1.05
1:A:147[A]:PHE:CD1	1:A:147[A]:PHE:CB	2.48	0.96
1:D:147[A]:PHE:CD1	1:D:147[A]:PHE:CB	2.48	0.96
1:C:147[A]:PHE:CB	1:C:147[A]:PHE:CD1	2.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1357:LDA:HM12	2:A:1373:LDA:CM2	1.99	0.92
2:A:1355:LDA:H42	2:A:1356:LDA:H31	1.58	0.86
2:A:1379:LDA:H52	2:A:1385:LDA:H51	1.57	0.84
1:A:279:LYS:CE	6:A:2475:HOH:O	2.27	0.83
1:A:279:LYS:HE2	6:A:2475:HOH:O	1.76	0.83
2:A:1366:LDA:HM12	2:A:1367:LDA:H51	1.62	0.81
1:A:174:TYR:HB2	2:A:1383:LDA:H92	1.65	0.78
2:A:1373:LDA:H11	2:A:1387:LDA:H42	1.66	0.78
2:A:1380:LDA:H11	2:A:1502:LDA:HM11	1.65	0.77
2:B:1360:LDA:H101	2:B:1373:LDA:H122	1.66	0.77
2:D:1354:LDA:H91	2:D:1362:LDA:H102	1.65	0.76
2:F:1366:LDA:H42	2:F:1504:LDA:H52	1.65	0.76
2:B:1366:LDA:H81	2:B:1372:LDA:H102	1.69	0.74
1:F:147:PHE:HB2	2:F:1365:LDA:H121	1.69	0.74
2:C:1351:LDA:H82	4:C:1370:MYR:H91	1.71	0.73
2:A:1350[B]:LDA:H72	2:A:1351:LDA:H51	1.71	0.73
3:C:1365:FTT:H141	2:C:1500:LDA:H111	1.70	0.72
2:F:1362:LDA:H62	2:F:1363:LDA:H52	1.71	0.72
2:F:1348:LDA:O1	6:F:2287:HOH:O	2.08	0.72
2:A:1387:LDA:H71	2:A:1388:LDA:H123	1.73	0.71
2:B:1366:LDA:HM11	2:B:1371:LDA:H72	1.73	0.70
2:B:1366:LDA:H12	2:B:1371:LDA:H81	1.74	0.69
1:D:297:VAL:HG12	2:D:1353:LDA:H82	1.75	0.69
1:B:136[A]:ASN:ND2	6:B:2292:HOH:O	2.25	0.69
2:A:1384:LDA:H51	2:A:1386:LDA:H72	1.75	0.69
2:F:1346:LDA:H21	2:F:1347:LDA:HM11	1.75	0.69
2:A:1358:LDA:H122	2:A:1372:LDA:H121	1.75	0.69
2:B:1348:LDA:H122	2:B:1353:LDA:H122	1.75	0.69
2:A:1374:LDA:H41	2:A:1502:LDA:H62	1.75	0.69
1:A:25:ASP:OD1	1:A:27:LYS:HG2	1.92	0.68
2:A:1366:LDA:H61	2:A:1368:LDA:H102	1.76	0.67
1:F:269:LEU:HD13	2:F:1352:LDA:H72	1.76	0.67
1:B:25:ASP:OD1	1:B:27:LYS:HG2	1.94	0.67
1:D:114:ASP:OD2	6:D:2303:HOH:O	2.12	0.67
2:F:1362:LDA:H11	2:F:1364:LDA:HM21	1.77	0.66
2:D:1346:LDA:H112	2:D:1356:LDA:H82	1.78	0.65
2:A:1377:LDA:H62	2:A:1383:LDA:H112	1.78	0.65
2:A:1379:LDA:H81	2:A:1386:LDA:H91	1.79	0.65
2:B:1501:LDA:O1	6:B:2544:HOH:O	2.15	0.65
2:A:1380:LDA:HM12	2:A:1387:LDA:H41	1.77	0.65
2:A:1369:LDA:H122	2:A:1379:LDA:H121	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1365:LDA:H52	2:F:1365:LDA:H91	1.79	0.64
1:C:143:ASP:OD1	6:C:2260:HOH:O	2.15	0.64
2:A:1355:LDA:H91	2:A:1388:LDA:H102	1.80	0.64
2:D:1357:LDA:HM23	2:F:1344:LDA:H22	1.80	0.63
2:F:1358:LDA:H42	2:F:1359:LDA:HM21	1.81	0.63
1:B:297:VAL:HG12	2:B:1344:LDA:H51	1.80	0.63
1:A:229:LEU:HB3	2:A:1387:LDA:H121	1.79	0.63
1:A:293:LYS:NZ	2:A:1354:LDA:HM12	2.14	0.62
2:A:1358:LDA:H122	2:A:1372:LDA:C12	2.29	0.62
1:A:147[A]:PHE:CD1	1:A:147[A]:PHE:HB3	2.33	0.62
1:E:25:ASP:OD1	1:E:27:LYS:HG2	1.99	0.61
1:F:297:VAL:HG12	2:F:1354:LDA:H123	1.82	0.61
2:F:1358:LDA:H61	2:F:1359:LDA:H11	1.82	0.61
2:B:1372:LDA:H31	2:B:1372:LDA:HM11	1.83	0.61
1:B:248:GLU:OE1	6:B:2420:HOH:O	2.16	0.61
1:A:273:ILE:HG23	2:A:1354:LDA:H122	1.83	0.61
2:D:1354:LDA:H32	2:D:1355:LDA:HM21	1.82	0.61
2:B:1354:LDA:HM23	2:B:1356:LDA:H72	1.82	0.60
2:B:1347:LDA:H41	2:B:1374:LDA:H41	1.82	0.60
1:A:68:THR:HG22	1:C:73:GLN:HG3	1.82	0.59
1:A:139:PHE:HD1	2:A:1365:LDA:H31	1.67	0.59
1:A:151:TYR:CE2	2:A:1376:LDA:H31	2.37	0.59
1:A:156:GLY:HA2	1:A:162:THR:HG22	1.84	0.59
1:F:89:LEU:HD23	2:F:1344:LDA:H92	1.83	0.58
2:F:1346:LDA:HM23	2:F:1347:LDA:HM13	1.86	0.58
2:B:1348:LDA:O1	6:B:2532:HOH:O	2.17	0.58
2:E:1347:LDA:H21	2:E:1347:LDA:H62	1.85	0.58
1:C:9:ASN:ND2	6:C:2024:HOH:O	2.37	0.57
2:E:1347:LDA:H32	2:E:1347:LDA:HM21	1.87	0.57
2:F:1502:LDA:H72	2:F:1504:LDA:H61	1.87	0.57
2:E:1357:LDA:H121	2:F:1351:LDA:H102	1.86	0.57
2:F:1352:LDA:H32	6:F:2338:HOH:O	2.05	0.57
2:E:1356:LDA:H101	2:E:1357:LDA:H82	1.87	0.56
1:C:293:LYS:NZ	2:C:1347:LDA:HM22	2.20	0.56
2:E:1357:LDA:H72	2:F:1351:LDA:H31	1.86	0.56
1:C:269:LEU:HD22	2:C:1360:LDA:H72	1.88	0.56
1:A:259:LEU:HD13	2:A:1387:LDA:H82	1.87	0.56
2:A:1354:LDA:H32	2:A:1355:LDA:H22	1.87	0.55
1:B:89:LEU:HD23	2:B:1365:LDA:H102	1.87	0.55
2:A:1346:LDA:H82	2:A:1357:LDA:H123	1.88	0.55
2:C:1351:LDA:H31	3:C:1369:FTT:H62	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1348:LDA:H111	2:E:1352:LDA:H111	1.89	0.55
1:E:49:ASP:HB2	1:E:50[B]:GLN:HE21	1.71	0.55
2:C:1347:LDA:H32	2:C:1352:LDA:HM12	1.89	0.54
2:B:1345:LDA:H31	2:B:1363:LDA:H42	1.89	0.54
1:C:273[A]:ILE:HD13	3:C:1369:FTT:H143	1.88	0.54
2:A:1354:LDA:H22	2:A:1387:LDA:HM12	1.90	0.54
1:B:182:LEU:HD22	2:B:1351:LDA:H61	1.88	0.54
2:A:1346:LDA:H121	2:A:1371:LDA:H121	1.89	0.53
1:D:85:ASP:HB3	2:D:1348:LDA:HM13	1.90	0.53
1:A:224:LEU:HD22	2:A:1350[B]:LDA:HM21	1.90	0.53
2:A:1384:LDA:H51	2:A:1386:LDA:H92	1.88	0.53
1:F:136:ASN:HD22	1:F:146:SER:HB2	1.73	0.53
2:A:1350[B]:LDA:H81	2:A:1375:LDA:H72	1.90	0.53
3:C:1365:FTT:H131	2:C:1500:LDA:H62	1.91	0.53
1:A:159:ASN:O	1:A:162:THR:HG23	2.08	0.53
2:A:1374:LDA:H21	2:A:1502:LDA:H42	1.91	0.53
1:C:86:TYR:CZ	2:C:1344:LDA:H32	2.44	0.53
2:D:1362:LDA:H32	2:D:1362:LDA:HM12	1.90	0.52
1:F:176:PHE:CE1	1:F:192:TYR:HB3	2.44	0.52
2:F:1351:LDA:H12	6:F:2338:HOH:O	2.10	0.52
1:A:224:LEU:HB3	2:A:1350[B]:LDA:HM21	1.91	0.52
1:E:333:ASN:HD21	2:E:1354:LDA:H11	1.74	0.52
2:A:1348:LDA:HM23	2:A:1350[B]:LDA:HM22	1.92	0.52
2:A:1354:LDA:HM23	2:A:1388:LDA:H32	1.92	0.52
2:D:1344:LDA:H41	2:D:1357:LDA:H11	1.92	0.52
2:B:1366:LDA:H102	2:B:1372:LDA:H123	1.91	0.52
2:D:1345:LDA:H22	2:D:1346:LDA:H31	1.91	0.52
2:D:1352:LDA:H121	2:D:1357:LDA:H101	1.90	0.52
1:E:154[B]:LYS:NZ	6:E:2287:HOH:O	2.42	0.52
1:F:81:LEU:HD12	2:F:1344:LDA:H82	1.92	0.51
2:F:1346:LDA:H82	2:F:1348:LDA:H101	1.92	0.51
1:A:275:TYR:HB2	2:A:1354:LDA:H92	1.91	0.51
1:D:174:TYR:HB2	2:D:1350:LDA:H62	1.92	0.51
2:A:1350[B]:LDA:H101	2:A:1375:LDA:H61	1.92	0.51
1:A:225:ASP:H	2:A:1350[B]:LDA:HM11	1.74	0.51
1:A:27:LYS:NZ	6:A:2070:HOH:O	2.44	0.51
2:F:1352:LDA:H21	2:F:1362:LDA:H31	1.92	0.51
2:B:1345:LDA:H21	2:B:1367:LDA:H51	1.93	0.50
1:A:186:LEU:HD11	2:A:1348:LDA:H101	1.93	0.50
2:A:1355:LDA:HM11	2:A:1355:LDA:H32	1.92	0.50
1:C:340:ILE:HD12	6:C:2450:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:LYS:NZ	6:D:2351:HOH:O	2.45	0.50
2:A:1357:LDA:O1	6:A:2576:HOH:O	2.19	0.50
1:B:81:LEU:HD12	2:B:1365:LDA:H92	1.93	0.50
1:C:52[A]:ILE:HG12	1:C:82:LYS:HE2	1.93	0.50
2:B:1362:LDA:H51	2:B:1363:LDA:H101	1.93	0.50
2:F:1353:LDA:HM23	2:F:1364:LDA:HM12	1.93	0.50
2:F:1359:LDA:H111	2:F:1360:LDA:H81	1.93	0.50
2:A:1350[B]:LDA:H122	2:A:1375:LDA:H32	1.94	0.50
2:C:1360:LDA:H31	2:C:1361:LDA:H52	1.92	0.50
1:A:338:GLY:N	6:A:2528:HOH:O	2.42	0.50
1:F:293:LYS:NZ	2:F:1345:LDA:HM23	2.27	0.49
2:A:1382:LDA:HM12	6:A:2376:HOH:O	2.11	0.49
2:B:1361:LDA:H51	2:B:1363:LDA:H72	1.94	0.49
2:C:1346:LDA:O1	6:C:2396:HOH:O	2.19	0.49
1:B:73:GLN:HG3	1:C:68:THR:HG22	1.93	0.49
1:E:253[B]:LYS:HB2	1:E:281:LYS:HB2	1.95	0.49
2:F:1358:LDA:H102	2:F:1360:LDA:H72	1.94	0.49
2:F:1355:LDA:H32	2:F:1366:LDA:HM23	1.93	0.49
2:A:1387:LDA:HM11	2:A:1388:LDA:H22	1.94	0.49
1:B:52[A]:ILE:HG12	1:B:82:LYS:HE2	1.92	0.49
2:C:1354:LDA:H31	2:C:1354:LDA:HM21	1.95	0.49
2:B:1354:LDA:HM11	2:B:1355:LDA:H42	1.94	0.49
3:C:1367:FTT:H61	4:C:1370:MYR:H121	1.94	0.49
2:F:1501:LDA:H42	2:F:1504:LDA:H32	1.95	0.49
1:A:275:TYR:CE1	2:A:1354:LDA:H52	2.48	0.49
2:B:1347:LDA:H32	2:B:1374:LDA:H21	1.95	0.49
2:C:1355:LDA:HM12	2:C:1501:LDA:H31	1.95	0.49
1:A:267:PHE:CD1	2:A:1362:LDA:H11	2.48	0.49
2:A:1384:LDA:H71	2:A:1386:LDA:H112	1.94	0.49
1:B:218:VAL:HG12	2:B:1350:LDA:H101	1.95	0.49
1:D:154:LYS:HE2	6:D:2353:HOH:O	2.11	0.49
2:B:1345:LDA:H82	2:B:1367:LDA:H122	1.95	0.48
6:A:2066:HOH:O	1:C:154:LYS:NZ	2.46	0.48
1:A:293:LYS:HZ1	2:A:1354:LDA:HM12	1.79	0.48
2:C:1355:LDA:HM21	2:C:1355:LDA:H31	1.96	0.48
2:D:1346:LDA:H92	2:D:1356:LDA:H51	1.96	0.48
2:F:1355:LDA:H41	2:F:1356:LDA:HM12	1.95	0.48
1:A:263:TYR:O	1:A:271:PRO:HD2	2.13	0.48
1:E:83:PHE:HE1	2:E:1356:LDA:H12	1.79	0.48
2:B:1373:LDA:H91	2:B:1501:LDA:C12	2.44	0.48
1:C:279:LYS:NZ	6:C:2400:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:LEU:HD23	2:D:1352:LDA:H41	1.95	0.48
2:A:1379:LDA:H72	2:A:1385:LDA:H71	1.95	0.47
2:A:1351:LDA:HM21	2:A:1351:LDA:H32	1.96	0.47
1:A:194:ASN:HB3	2:A:1383:LDA:H82	1.96	0.47
1:B:271:PRO:HG3	2:B:1368:LDA:H61	1.96	0.47
1:F:303:PHE:HE1	2:F:1351:LDA:H52	1.79	0.47
1:A:118:GLN:NE2	6:A:2292:HOH:O	2.47	0.47
2:F:1501:LDA:H41	2:F:1504:LDA:H51	1.97	0.47
2:C:1352:LDA:H51	2:C:1501:LDA:H62	1.94	0.47
1:A:73:GLN:HG3	1:B:68:THR:HG22	1.97	0.47
1:F:189:GLY:HA2	2:F:1349:LDA:H123	1.97	0.47
1:F:301:TYR:CD1	2:F:1352:LDA:H71	2.49	0.47
2:B:1351:LDA:H112	2:B:1353:LDA:H112	1.97	0.47
2:B:1371:LDA:H81	2:B:1371:LDA:H112	1.63	0.47
2:B:1359:LDA:H92	2:B:1500:LDA:H112	1.96	0.47
1:D:310:VAL:HG22	6:D:2531:HOH:O	2.15	0.46
2:F:1357:LDA:H82	2:F:1358:LDA:C12	2.45	0.46
1:E:307:MET:CE	1:E:341:TYR:HD1	2.29	0.46
2:F:1365:LDA:O1	2:F:1366:LDA:H11	2.15	0.46
2:F:1351:LDA:H121	6:F:2384:HOH:O	2.14	0.46
1:E:263:TYR:O	1:E:271:PRO:HD2	2.16	0.46
1:E:83:PHE:CE1	2:E:1356:LDA:H12	2.51	0.46
2:B:1359:LDA:H22	2:B:1371:LDA:H41	1.98	0.46
2:C:1357:LDA:H92	2:C:1360:LDA:H123	1.96	0.46
1:C:25:ASP:OD1	1:C:27:LYS:HG2	2.15	0.46
2:A:1357:LDA:H31	2:A:1358:LDA:H61	1.96	0.46
2:B:1360:LDA:H81	2:B:1373:LDA:H101	1.99	0.46
1:C:293:LYS:HZ1	2:C:1347:LDA:HM22	1.80	0.46
1:C:263:TYR:O	1:C:271:PRO:HD2	2.16	0.45
1:F:303:PHE:CE1	2:F:1351:LDA:H52	2.51	0.45
1:E:52[A]:ILE:HG12	1:E:82:LYS:HE2	1.98	0.45
2:A:1367:LDA:HM23	2:A:1367:LDA:H21	1.72	0.45
2:B:1369:LDA:HM21	2:B:1369:LDA:H31	1.98	0.45
1:D:49:ASP:HB2	1:D:50[B]:GLN:HE21	1.80	0.45
2:E:1349:LDA:HM11	2:E:1349:LDA:H21	1.73	0.45
1:D:301:TYR:OH	2:D:1344:LDA:H11	2.16	0.45
1:A:218:VAL:HG12	2:A:1370:LDA:H91	1.97	0.45
1:B:234:GLY:N	6:B:2264:HOH:O	2.50	0.45
1:B:263:TYR:O	1:B:271:PRO:HD2	2.16	0.45
1:D:7:ASP:HA	6:D:2021:HOH:O	2.17	0.45
1:E:333:ASN:ND2	2:E:1354:LDA:H11	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1346:LDA:H61	2:A:1346:LDA:H92	1.59	0.45
2:E:1344:LDA:H82	2:E:1345:LDA:H31	1.99	0.45
1:F:297:VAL:HG11	2:F:1357:LDA:H51	1.98	0.45
2:A:1354:LDA:HM22	2:A:1388:LDA:H11	1.98	0.45
2:D:1346:LDA:H72	2:D:1356:LDA:H42	1.98	0.45
1:B:232:MET:HE3	6:B:2264:HOH:O	2.16	0.45
2:F:1352:LDA:H21	2:F:1362:LDA:C3	2.46	0.45
1:F:203:ASN:HB2	1:F:209:THR:HG22	1.99	0.45
2:F:1349:LDA:H12	2:F:1500:LDA:HM23	1.99	0.44
1:A:337:LEU:HD22	6:A:2257:HOH:O	2.18	0.44
1:C:109:PRO:HB3	1:C:310:VAL:HB	1.98	0.44
1:A:8:GLY:O	6:A:2018:HOH:O	2.21	0.44
1:E:203:ASN:HB2	1:E:209:THR:HG22	1.99	0.44
2:F:1500:LDA:HM12	2:F:1504:LDA:HM11	2.00	0.44
1:A:261:ALA:C	1:A:262:LEU:HD12	2.38	0.44
2:F:1366:LDA:HM12	2:F:1366:LDA:H22	1.79	0.44
2:C:1352:LDA:H11	2:C:1501:LDA:HM12	1.99	0.44
1:B:131:LEU:HD22	2:C:1358:LDA:H52	2.00	0.44
4:C:1364:MYR:H52	4:C:1364:MYR:H82	1.81	0.44
1:C:145:LEU:O	6:C:2254:HOH:O	2.21	0.44
1:C:158[A]:GLN:HG2	6:C:2269:HOH:O	2.17	0.44
2:D:1357:LDA:HM23	2:F:1344:LDA:HM21	1.99	0.44
1:B:109[B]:PRO:HB3	1:B:310:VAL:HB	1.99	0.44
1:D:263:TYR:OH	2:D:1362:LDA:HM21	2.18	0.43
1:D:263:TYR:O	1:D:271:PRO:HD2	2.18	0.43
1:E:144:GLY:N	6:E:2275:HOH:O	2.38	0.43
1:E:154[B]:LYS:NZ	6:E:2288:HOH:O	2.35	0.43
2:D:1345:LDA:H91	2:D:1356:LDA:H81	2.00	0.43
2:B:1372:LDA:HM21	2:B:1373:LDA:H61	2.00	0.43
2:B:1373:LDA:H91	2:B:1501:LDA:H123	2.00	0.43
1:B:109[A]:PRO:HB3	1:B:310:VAL:HB	2.00	0.43
2:A:1368:LDA:H21	2:A:1369:LDA:HM23	2.01	0.43
1:E:315:ILE:HD13	2:E:1355:LDA:H91	1.99	0.43
1:B:136[B]:ASN:C	1:B:136[B]:ASN:HD22	2.22	0.43
1:F:109:PRO:HB3	1:F:310:VAL:HB	2.01	0.43
2:F:1358:LDA:H32	2:F:1360:LDA:HM23	2.01	0.43
2:A:1359:LDA:H72	1:C:91:TYR:CD2	2.52	0.43
2:D:1360:LDA:H31	2:D:1360:LDA:H62	1.56	0.43
2:A:1357:LDA:H81	2:A:1374:LDA:H71	2.01	0.42
2:A:1387:LDA:HM11	2:A:1388:LDA:C3	2.49	0.42
1:D:261:ALA:C	1:D:262:LEU:HD12	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:ILE:HD12	6:D:2531:HOH:O	2.18	0.42
2:A:1380:LDA:HM12	2:A:1387:LDA:C4	2.48	0.42
1:E:49:ASP:HB2	1:E:50[B]:GLN:NE2	2.34	0.42
2:C:1360:LDA:H41	2:C:1361:LDA:H72	2.01	0.42
1:C:305[B]:LYS:NZ	6:C:2448:HOH:O	2.52	0.42
1:A:136[A]:ASN:ND2	6:A:2321:HOH:O	2.51	0.42
1:A:279:LYS:HE3	6:A:2475:HOH:O	2.05	0.42
2:C:1352:LDA:H31	2:C:1501:LDA:H42	2.01	0.42
1:C:192:TYR:CZ	3:C:1365:FTT:H51	2.55	0.42
1:C:314:LYS:NZ	6:C:2452:HOH:O	2.51	0.42
1:E:174:TYR:HB2	2:E:1346:LDA:H61	2.02	0.42
2:A:1368:LDA:H31	2:A:1368:LDA:HM12	2.01	0.42
2:B:1371:LDA:HM23	2:B:1371:LDA:H32	2.01	0.42
2:D:1354:LDA:HM12	2:D:1354:LDA:H31	2.02	0.42
1:D:263:TYR:CD2	2:D:1354:LDA:H42	2.55	0.42
2:E:1344:LDA:H21	2:E:1344:LDA:HM23	1.83	0.42
2:A:1382:LDA:HM11	2:A:1383:LDA:H21	2.02	0.42
1:A:141:TYR:O	2:A:1385:LDA:H12	2.19	0.42
2:C:1501:LDA:H22	2:C:1501:LDA:HM21	1.76	0.42
3:C:1365:FTT:H91	4:C:1366:MYR:H52	2.02	0.42
1:C:192:TYR:HD1	1:C:216:TRP:HB3	1.85	0.42
1:D:314:LYS:NZ	6:D:2535:HOH:O	2.53	0.42
2:F:1355:LDA:H51	2:F:1365:LDA:H12	2.02	0.42
1:A:313:TYR:CE1	2:A:1353:LDA:HM12	2.55	0.41
2:B:1373:LDA:H22	2:B:1373:LDA:HM12	1.84	0.41
1:E:212:ARG:CZ	2:E:1346:LDA:HM21	2.50	0.41
2:A:1367:LDA:H12	2:A:1368:LDA:HM12	2.02	0.41
1:C:233:TYR:HB2	2:C:1345:LDA:H52	2.01	0.41
2:A:1357:LDA:H61	2:A:1374:LDA:H51	2.02	0.41
2:F:1358:LDA:H42	2:F:1359:LDA:H11	2.02	0.41
1:F:338:GLY:N	6:F:2384:HOH:O	2.52	0.41
2:A:1379:LDA:H32	2:A:1385:LDA:H42	2.02	0.41
2:C:1351:LDA:H51	3:C:1369:FTT:H81	2.02	0.41
1:E:307:MET:HE2	1:E:341:TYR:HD1	1.86	0.41
2:F:1344:LDA:HM11	2:F:1344:LDA:H21	1.69	0.41
2:A:1366:LDA:O1	2:A:1370:LDA:H41	2.21	0.41
1:A:212:ARG:HD2	2:A:1383:LDA:HM12	2.03	0.41
2:C:1352:LDA:H52	2:C:1353:LDA:H101	2.03	0.41
2:D:1344:LDA:H42	2:F:1344:LDA:H21	2.03	0.41
2:D:1355:LDA:HM11	2:D:1355:LDA:H21	1.82	0.41
2:F:1346:LDA:H21	2:F:1347:LDA:CM1	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1368:MYR:H42	4:C:1368:MYR:H71	1.89	0.41
1:C:156:GLY:HA2	1:C:162:THR:OG1	2.21	0.41
2:B:1371:LDA:H51	2:B:1372:LDA:HM12	2.03	0.41
2:D:1356:LDA:H21	2:D:1357:LDA:HM12	2.03	0.41
2:A:1376:LDA:H123	2:B:1345:LDA:H123	2.04	0.40
2:F:1348:LDA:H61	2:F:1350:LDA:H51	2.03	0.40
2:A:1349:LDA:H71	2:A:1349:LDA:H41	1.91	0.40
2:B:1348:LDA:CM2	2:B:1349:LDA:H11	2.51	0.40
2:C:1352:LDA:H12	2:C:1353:LDA:H62	2.03	0.40
1:E:91:TYR:CD2	2:E:1344:LDA:H123	2.57	0.40
2:F:1362:LDA:H102	2:F:1362:LDA:H71	1.79	0.40
2:F:1365:LDA:H22	2:F:1365:LDA:HM12	1.87	0.40
1:A:184:TRP:HA	2:A:1348:LDA:H12	2.01	0.40
1:A:184:TRP:CZ2	2:A:1347:LDA:H42	2.56	0.40
1:A:224:LEU:HD22	2:A:1350[B]:LDA:CM2	2.52	0.40
2:B:1366:LDA:H123	2:B:1374:LDA:H62	2.04	0.40
2:C:1359:LDA:H12	4:C:1366:MYR:H72	2.03	0.40
1:C:95:TYR:HE1	6:C:2156:HOH:O	2.02	0.40
2:D:1346:LDA:H21	2:D:1346:LDA:HM11	1.88	0.40
2:D:1352:LDA:H22	2:D:1352:LDA:HM21	1.87	0.40
1:D:151:TYR:CE2	2:D:1347:LDA:H32	2.57	0.40
2:F:1352:LDA:H42	2:F:1362:LDA:H51	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	345/343 (101%)	334 (97%)	11 (3%)	0	100	100
1	B	349/343 (102%)	334 (96%)	14 (4%)	1 (0%)	44	49
1	C	349/343 (102%)	337 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	346/343 (101%)	334 (96%)	12 (4%)	0	100	100
1	E	349/343 (102%)	334 (96%)	15 (4%)	0	100	100
1	F	344/343 (100%)	332 (96%)	12 (4%)	0	100	100
All	All	2082/2058 (101%)	2005 (96%)	76 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	ASP

### 5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	280/276 (101%)	266 (95%)	14 (5%)	28	34
1	B	284/276 (103%)	274 (96%)	10 (4%)	41	51
1	C	284/276 (103%)	269 (95%)	15 (5%)	26	31
1	D	281/276 (102%)	270 (96%)	11 (4%)	37	46
1	E	284/276 (103%)	272 (96%)	12 (4%)	34	43
1	F	279/276 (101%)	268 (96%)	11 (4%)	37	46
All	All	1692/1656 (102%)	1619 (96%)	73 (4%)	40	41

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	42	LYS
1	A	50[A]	GLN
1	A	50[B]	GLN
1	A	85	ASP
1	A	128	ARG
1	A	137	ASN

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Mol	Chain	Res	Type
1	A	158[A]	GLN
1	A	158[B]	GLN
1	A	162	THR
1	A	167	LEU
1	A	227	LEU
1	A	276	ASN
1	A	291	LEU
1	B	36	ARG
1	B	50[A]	GLN
1	B	50[B]	GLN
1	B	52[A]	ILE
1	B	52[B]	ILE
1	B	128	ARG
1	B	227	LEU
1	B	254	THR
1	B	276	ASN
1	B	291	LEU
1	C	27	LYS
1	C	36	ARG
1	C	50[A]	GLN
1	C	50[B]	GLN
1	C	52[A]	ILE
1	C	52[B]	ILE
1	C	73	GLN
1	C	128	ARG
1	C	137	ASN
1	C	147[A]	PHE
1	C	147[B]	PHE
1	C	167	LEU
1	C	227	LEU
1	C	276	ASN
1	C	291	LEU
1	D	36	ARG
1	D	128	ARG
1	D	147[A]	PHE
1	D	147[B]	PHE
1	D	154	LYS
1	D	158[A]	GLN
1	D	158[B]	GLN
1	D	227	LEU
1	D	237	LEU
1	D	276	ASN

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Mol	Chain	Res	Type
1	D	291	LEU
1	E	36	ARG
1	E	52[A]	ILE
1	E	52[B]	ILE
1	E	128	ARG
1	E	149	LEU
1	E	154[A]	LYS
1	E	154[B]	LYS
1	E	227	LEU
1	E	237[A]	LEU
1	E	237[B]	LEU
1	E	276	ASN
1	E	291	LEU
1	F	27	LYS
1	F	36	ARG
1	F	50[A]	GLN
1	F	50[B]	GLN
1	F	128	ARG
1	F	149	LEU
1	F	227	LEU
1	F	237	LEU
1	F	276	ASN
1	F	291	LEU
1	F	337	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	B	256	ASN
1	E	21	HIS
1	F	136	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

180 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	LDA	A	1344	-	13,15,15	0.87	1 (7%)	14,17,17	0.74	0
2	LDA	A	1345	-	13,15,15	0.74	0	14,17,17	0.96	1 (7%)
2	LDA	A	1346	-	13,15,15	0.71	1 (7%)	14,17,17	1.06	2 (14%)
2	LDA	A	1347	-	13,15,15	0.76	0	14,17,17	0.82	0
2	LDA	A	1348	-	13,15,15	0.79	1 (7%)	14,17,17	0.49	0
2	LDA	A	1349	-	13,15,15	0.84	1 (7%)	14,17,17	0.73	0
2	LDA	A	1350[A]	-	13,15,15	0.81	1 (7%)	14,17,17	0.53	0
2	LDA	A	1350[B]	-	13,15,15	0.92	1 (7%)	14,17,17	0.77	0
2	LDA	A	1351	-	11,13,15	0.80	1 (9%)	12,15,17	1.08	1 (8%)
2	LDA	A	1352	-	9,11,15	0.95	1 (11%)	10,13,17	0.47	0
2	LDA	A	1353	-	8,10,15	1.05	1 (12%)	9,12,17	0.59	0
2	LDA	A	1354	-	13,15,15	0.78	0	14,17,17	1.02	0
2	LDA	A	1355	-	13,15,15	0.80	1 (7%)	14,17,17	1.01	1 (7%)
2	LDA	A	1356	-	8,10,15	1.06	1 (12%)	9,12,17	0.47	0
2	LDA	A	1357	-	13,15,15	0.87	1 (7%)	14,17,17	0.87	1 (7%)
2	LDA	A	1358	-	13,15,15	2.47	2 (15%)	14,17,17	0.55	0
2	LDA	A	1359	-	7,7,15	0.30	0	6,6,17	0.51	0
2	LDA	A	1360	-	9,11,15	0.93	0	10,13,17	1.83	3 (30%)
2	LDA	A	1361	-	13,15,15	0.80	1 (7%)	14,17,17	0.89	1 (7%)
2	LDA	A	1362	-	13,15,15	0.91	1 (7%)	14,17,17	0.74	0
2	LDA	A	1363	-	8,8,15	0.39	0	7,7,17	0.51	0
2	LDA	A	1364	-	8,8,15	0.32	0	7,7,17	0.53	0
2	LDA	A	1365	-	13,15,15	0.87	1 (7%)	14,17,17	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LDA	A	1366	-	13,15,15	0.68	0	14,17,17	1.02	1 (7%)
2	LDA	A	1367	-	13,15,15	0.78	1 (7%)	14,17,17	1.18	1 (7%)
2	LDA	A	1368	-	13,15,15	0.86	1 (7%)	14,17,17	1.50	3 (21%)
2	LDA	A	1369	-	13,15,15	0.82	1 (7%)	14,17,17	0.62	0
2	LDA	A	1370	-	13,15,15	0.86	1 (7%)	14,17,17	1.15	1 (7%)
2	LDA	A	1371	-	13,15,15	0.84	1 (7%)	14,17,17	0.61	0
2	LDA	A	1372	-	13,15,15	0.81	0	14,17,17	0.68	0
2	LDA	A	1373	-	13,15,15	2.49	2 (15%)	14,17,17	0.55	0
2	LDA	A	1374	-	7,7,15	0.31	0	6,6,17	0.55	0
2	LDA	A	1375	-	8,8,15	0.37	0	7,7,17	0.48	0
2	LDA	A	1376	-	13,15,15	0.89	1 (7%)	14,17,17	0.62	0
2	LDA	A	1377	-	13,15,15	0.82	1 (7%)	14,17,17	0.57	0
2	LDA	A	1378	-	8,8,15	0.33	0	7,7,17	0.55	0
2	LDA	A	1379	-	13,15,15	0.83	1 (7%)	14,17,17	0.68	0
2	LDA	A	1380	-	8,10,15	1.04	1 (12%)	9,12,17	0.64	0
2	LDA	A	1381	-	13,15,15	0.80	1 (7%)	14,17,17	0.56	0
2	LDA	A	1382	-	13,15,15	0.84	1 (7%)	14,17,17	0.80	0
2	LDA	A	1383	-	13,15,15	0.84	1 (7%)	14,17,17	0.69	0
2	LDA	A	1384	-	13,15,15	0.83	1 (7%)	14,17,17	0.76	0
2	LDA	A	1385	-	13,15,15	0.83	1 (7%)	14,17,17	0.71	0
2	LDA	A	1386	-	13,15,15	0.90	1 (7%)	14,17,17	0.73	0
2	LDA	A	1387	-	13,15,15	0.73	0	14,17,17	1.73	3 (21%)
2	LDA	A	1388	-	13,15,15	0.94	1 (7%)	14,17,17	1.10	1 (7%)
2	LDA	A	1500	-	10,10,15	0.38	0	9,9,17	0.63	0
2	LDA	A	1501	-	8,10,15	1.09	1 (12%)	9,12,17	0.53	0
2	LDA	A	1502	-	8,10,15	1.02	1 (12%)	9,12,17	0.60	0
2	LDA	B	1344	-	7,9,15	1.04	1 (14%)	8,11,17	0.51	0
2	LDA	B	1345	-	13,15,15	0.83	1 (7%)	14,17,17	0.60	0
2	LDA	B	1346	-	13,15,15	0.81	1 (7%)	14,17,17	0.72	0
2	LDA	B	1347	-	13,15,15	0.71	0	14,17,17	0.85	0
2	LDA	B	1348	-	13,15,15	0.81	0	14,17,17	1.05	1 (7%)
2	LDA	B	1349	-	10,12,15	0.96	1 (10%)	11,14,17	0.51	0
2	LDA	B	1350	-	13,15,15	0.91	1 (7%)	14,17,17	0.86	0
2	LDA	B	1351	-	13,15,15	0.78	0	14,17,17	1.00	1 (7%)
2	LDA	B	1352	-	13,15,15	0.82	1 (7%)	14,17,17	0.90	0
2	LDA	B	1353	-	13,15,15	0.81	1 (7%)	14,17,17	0.93	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LDA	B	1354	-	13,15,15	0.84	1 (7%)	14,17,17	0.69	0
2	LDA	B	1355	-	13,15,15	0.83	1 (7%)	14,17,17	0.57	0
2	LDA	B	1356	-	13,15,15	0.78	0	14,17,17	0.51	0
2	LDA	B	1357	-	8,8,15	0.32	0	7,7,17	0.53	0
2	LDA	B	1358	-	9,11,15	0.86	0	10,13,17	0.51	0
2	LDA	B	1359	-	13,15,15	0.86	1 (7%)	14,17,17	0.69	0
2	LDA	B	1360	-	13,15,15	0.92	1 (7%)	14,17,17	0.74	0
2	LDA	B	1361	-	8,8,15	0.36	0	7,7,17	0.52	0
2	LDA	B	1362	-	8,8,15	0.37	0	7,7,17	0.46	0
2	LDA	B	1363	-	13,15,15	0.83	1 (7%)	14,17,17	0.71	0
2	LDA	B	1364	-	13,15,15	0.89	1 (7%)	14,17,17	0.69	0
2	LDA	B	1365	-	13,15,15	0.80	1 (7%)	14,17,17	0.70	0
2	LDA	B	1366	-	13,15,15	0.85	1 (7%)	14,17,17	1.75	5 (35%)
2	LDA	B	1367	-	13,15,15	0.78	1 (7%)	14,17,17	0.77	0
2	LDA	B	1368	-	8,10,15	0.99	1 (12%)	9,12,17	0.51	0
2	LDA	B	1369	-	13,15,15	0.79	1 (7%)	14,17,17	1.07	1 (7%)
2	LDA	B	1370	-	5,7,15	1.25	1 (20%)	6,9,17	0.59	0
2	LDA	B	1371	-	13,15,15	0.81	1 (7%)	14,17,17	1.64	4 (28%)
2	LDA	B	1372	-	13,15,15	0.77	1 (7%)	14,17,17	1.53	1 (7%)
2	LDA	B	1373	-	13,15,15	0.77	1 (7%)	14,17,17	0.64	0
2	LDA	B	1374	-	13,15,15	0.88	1 (7%)	14,17,17	1.05	1 (7%)
3	FTT	B	1375	4	15,15,16	1.06	2 (13%)	15,15,17	0.98	1 (6%)
4	MYR	B	1376	3	14,14,15	0.49	0	13,13,15	1.07	1 (7%)
2	LDA	B	1500	-	13,15,15	0.83	1 (7%)	14,17,17	0.61	0
2	LDA	B	1501	-	13,15,15	0.78	1 (7%)	14,17,17	0.66	0
2	LDA	C	1344	-	13,15,15	0.84	1 (7%)	14,17,17	0.57	0
2	LDA	C	1345	-	13,15,15	0.88	2 (15%)	14,17,17	0.84	0
2	LDA	C	1346	-	13,15,15	0.82	1 (7%)	14,17,17	0.69	0
2	LDA	C	1347	-	13,15,15	0.84	1 (7%)	14,17,17	3.14	4 (28%)
2	LDA	C	1348	-	8,10,15	1.11	1 (12%)	9,12,17	0.55	0
2	LDA	C	1349	-	5,7,15	1.24	1 (20%)	6,9,17	0.42	0
2	LDA	C	1350	-	13,15,15	0.81	1 (7%)	14,17,17	0.62	0
2	LDA	C	1351	-	13,15,15	0.80	1 (7%)	14,17,17	0.62	0
2	LDA	C	1352	-	8,10,15	0.97	1 (12%)	9,12,17	0.46	0
2	LDA	C	1353	-	13,15,15	0.79	1 (7%)	14,17,17	0.53	0
2	LDA	C	1354	-	8,10,15	0.99	1 (12%)	9,12,17	1.09	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LDA	C	1355	-	6,8,15	1.12	1 (16%)	7,10,17	1.27	1 (14%)
2	LDA	C	1356	-	13,15,15	0.82	1 (7%)	14,17,17	0.62	0
2	LDA	C	1357	-	13,15,15	0.87	1 (7%)	14,17,17	1.08	0
2	LDA	C	1358	-	9,9,15	0.32	0	8,8,17	0.54	0
2	LDA	C	1359	-	8,10,15	1.14	1 (12%)	9,12,17	1.09	0
2	LDA	C	1360	-	13,15,15	0.89	1 (7%)	14,17,17	0.96	0
2	LDA	C	1361	-	13,15,15	0.85	1 (7%)	14,17,17	0.61	0
2	LDA	C	1362	-	13,15,15	0.83	1 (7%)	14,17,17	0.72	0
3	FTT	C	1363	4	15,15,16	1.02	1 (6%)	15,15,17	1.18	2 (13%)
4	MYR	C	1364	3	14,14,15	0.47	0	13,13,15	0.84	0
3	FTT	C	1365	4	15,15,16	1.00	1 (6%)	15,15,17	1.08	2 (13%)
4	MYR	C	1366	3	14,14,15	0.46	0	13,13,15	0.83	0
3	FTT	C	1367	4	15,15,16	1.03	1 (6%)	15,15,17	1.08	2 (13%)
4	MYR	C	1368	3	14,14,15	0.44	0	13,13,15	0.82	0
3	FTT	C	1369	4	15,15,16	1.00	1 (6%)	15,15,17	1.11	2 (13%)
4	MYR	C	1370	3	14,14,15	0.46	0	13,13,15	0.86	0
5	SO4	C	1371	-	4,4,4	0.17	0	6,6,6	0.09	0
2	LDA	C	1500	-	13,15,15	0.75	0	14,17,17	0.65	0
2	LDA	C	1501	-	8,10,15	0.86	0	9,12,17	1.10	1 (11%)
2	LDA	C	1502	-	7,7,15	0.34	0	6,6,17	0.52	0
2	LDA	D	1344	-	13,15,15	0.81	0	14,17,17	0.85	0
2	LDA	D	1345	-	13,15,15	0.80	1 (7%)	14,17,17	0.61	0
2	LDA	D	1346	-	13,15,15	0.84	1 (7%)	14,17,17	0.57	0
2	LDA	D	1347	-	13,15,15	0.84	1 (7%)	14,17,17	1.22	2 (14%)
2	LDA	D	1348	-	13,15,15	0.83	1 (7%)	14,17,17	0.94	0
2	LDA	D	1349	-	13,15,15	0.80	0	14,17,17	0.65	0
2	LDA	D	1350	-	8,10,15	1.19	1 (12%)	9,12,17	0.53	0
2	LDA	D	1351	-	8,10,15	1.09	1 (12%)	9,12,17	0.55	0
2	LDA	D	1352	-	13,15,15	0.81	1 (7%)	14,17,17	0.80	0
2	LDA	D	1353	-	13,15,15	0.87	1 (7%)	14,17,17	1.02	2 (14%)
2	LDA	D	1354	-	11,13,15	0.77	0	12,15,17	1.46	3 (25%)
2	LDA	D	1355	-	13,15,15	0.79	1 (7%)	14,17,17	0.70	0
2	LDA	D	1356	-	13,15,15	0.83	1 (7%)	14,17,17	0.54	0
2	LDA	D	1357	-	13,15,15	0.84	1 (7%)	14,17,17	0.70	0
2	LDA	D	1358	-	7,7,15	0.37	0	6,6,17	0.42	0
2	LDA	D	1359	-	7,7,15	0.36	0	6,6,17	0.47	0
2	LDA	D	1360	-	13,15,15	0.77	1 (7%)	14,17,17	1.10	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LDA	D	1361	-	7,7,15	0.27	0	6,6,17	0.58	0
2	LDA	D	1362	-	13,15,15	0.74	1 (7%)	14,17,17	1.60	2 (14%)
2	LDA	D	1363	-	13,15,15	0.82	1 (7%)	14,17,17	1.12	2 (14%)
3	FTT	D	1364	4	15,15,16	1.00	1 (6%)	15,15,17	1.03	2 (13%)
4	MYR	D	1365	3	14,14,15	0.51	0	13,13,15	1.00	1 (7%)
5	SO4	D	1366	-	4,4,4	0.17	0	6,6,6	0.07	0
2	LDA	E	1344	-	13,15,15	0.81	1 (7%)	14,17,17	0.88	0
2	LDA	E	1345	-	8,10,15	1.01	1 (12%)	9,12,17	0.60	0
2	LDA	E	1346	-	8,10,15	0.98	1 (12%)	9,12,17	0.61	0
2	LDA	E	1347	-	8,10,15	1.06	1 (12%)	9,12,17	1.51	1 (11%)
2	LDA	E	1348	-	13,15,15	0.83	1 (7%)	14,17,17	0.85	0
2	LDA	E	1349	-	11,13,15	0.81	1 (9%)	12,15,17	0.72	0
2	LDA	E	1350	-	13,15,15	0.81	1 (7%)	14,17,17	0.55	0
2	LDA	E	1351	-	8,10,15	1.08	1 (12%)	9,12,17	0.47	0
2	LDA	E	1352	-	13,15,15	1.03	1 (7%)	14,17,17	0.99	0
2	LDA	E	1353	-	9,9,15	0.35	0	8,8,17	0.91	0
2	LDA	E	1354	-	13,15,15	0.86	1 (7%)	14,17,17	0.66	0
2	LDA	E	1355	-	13,15,15	0.89	1 (7%)	14,17,17	0.74	0
2	LDA	E	1356	-	13,15,15	0.83	1 (7%)	14,17,17	0.64	0
2	LDA	E	1357	-	13,15,15	0.93	1 (7%)	14,17,17	0.89	0
2	LDA	F	1344	-	13,15,15	0.71	0	14,17,17	1.01	1 (7%)
2	LDA	F	1345	-	13,15,15	0.82	1 (7%)	14,17,17	0.69	0
2	LDA	F	1346	-	13,15,15	0.80	1 (7%)	14,17,17	0.79	0
2	LDA	F	1347	-	13,15,15	0.68	0	14,17,17	0.65	0
2	LDA	F	1348	-	13,15,15	0.75	0	14,17,17	0.87	0
2	LDA	F	1349	-	13,15,15	0.80	1 (7%)	14,17,17	0.82	0
2	LDA	F	1350	-	13,15,15	0.88	1 (7%)	14,17,17	0.84	0
2	LDA	F	1351	-	13,15,15	0.89	2 (15%)	14,17,17	1.08	1 (7%)
2	LDA	F	1352	-	13,15,15	0.87	1 (7%)	14,17,17	0.96	0
2	LDA	F	1353	-	13,15,15	0.82	1 (7%)	14,17,17	0.62	0
2	LDA	F	1354	-	13,15,15	0.81	1 (7%)	14,17,17	0.64	0
2	LDA	F	1355	-	8,10,15	0.89	0	9,12,17	0.42	0
2	LDA	F	1356	-	8,10,15	0.89	0	9,12,17	0.51	0
2	LDA	F	1357	-	13,15,15	0.87	1 (7%)	14,17,17	0.85	0
2	LDA	F	1358	-	13,15,15	0.85	1 (7%)	14,17,17	0.86	0
2	LDA	F	1359	-	13,15,15	0.81	1 (7%)	14,17,17	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LDA	F	1360	-	13,15,15	0.87	1 (7%)	14,17,17	0.64	0
2	LDA	F	1361	-	13,15,15	0.88	1 (7%)	14,17,17	0.68	0
2	LDA	F	1362	-	13,15,15	0.87	1 (7%)	14,17,17	0.88	0
2	LDA	F	1363	-	13,15,15	0.87	1 (7%)	14,17,17	0.87	0
2	LDA	F	1364	-	13,15,15	0.78	0	14,17,17	1.12	1 (7%)
2	LDA	F	1365	-	13,15,15	0.82	1 (7%)	14,17,17	0.99	1 (7%)
2	LDA	F	1366	-	13,15,15	0.78	1 (7%)	14,17,17	0.97	0
2	LDA	F	1500	-	9,11,15	1.08	1 (11%)	10,13,17	0.91	1 (10%)
2	LDA	F	1501	-	13,15,15	0.84	1 (7%)	14,17,17	0.75	0
2	LDA	F	1502	-	9,9,15	0.32	0	8,8,17	0.65	0
2	LDA	F	1503	-	13,15,15	0.78	1 (7%)	14,17,17	0.57	0
2	LDA	F	1504	-	13,15,15	0.72	0	14,17,17	3.89	8 (57%)

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
2	LDA	A	1344	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1345	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1346	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1347	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1348	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1349	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1350[A]	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1350[B]	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1351	-	-	0/11/11/13	0/0/0/0
2	LDA	A	1352	-	-	0/9/9/13	0/0/0/0
2	LDA	A	1353	-	-	0/8/8/13	0/0/0/0
2	LDA	A	1354	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1355	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1356	-	-	0/8/8/13	0/0/0/0
2	LDA	A	1357	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1358	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1359	-	-	0/5/5/13	0/0/0/0
2	LDA	A	1360	-	-	0/9/9/13	0/0/0/0
2	LDA	A	1361	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1362	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1363	-	-	0/6/6/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LDA	A	1364	-	-	0/6/6/13	0/0/0/0
2	LDA	A	1365	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1366	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1367	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1368	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1369	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1370	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1371	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1372	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1373	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1374	-	-	0/5/5/13	0/0/0/0
2	LDA	A	1375	-	-	0/6/6/13	0/0/0/0
2	LDA	A	1376	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1377	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1378	-	-	0/6/6/13	0/0/0/0
2	LDA	A	1379	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1380	-	-	0/8/8/13	0/0/0/0
2	LDA	A	1381	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1382	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1383	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1384	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1385	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1386	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1387	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1388	-	-	0/13/13/13	0/0/0/0
2	LDA	A	1500	-	-	0/8/8/13	0/0/0/0
2	LDA	A	1501	-	-	0/8/8/13	0/0/0/0
2	LDA	A	1502	-	-	0/8/8/13	0/0/0/0
2	LDA	B	1344	-	-	0/7/7/13	0/0/0/0
2	LDA	B	1345	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1346	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1347	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1348	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1349	-	-	0/10/10/13	0/0/0/0
2	LDA	B	1350	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1351	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1352	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1353	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1354	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1355	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1356	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1357	-	-	0/6/6/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LDA	B	1358	-	-	0/9/9/13	0/0/0/0
2	LDA	B	1359	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1360	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1361	-	-	0/6/6/13	0/0/0/0
2	LDA	B	1362	-	-	0/6/6/13	0/0/0/0
2	LDA	B	1363	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1364	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1365	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1366	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1367	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1368	-	-	0/8/8/13	0/0/0/0
2	LDA	B	1369	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1370	-	-	0/5/5/13	0/0/0/0
2	LDA	B	1371	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1372	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1373	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1374	-	-	0/13/13/13	0/0/0/0
3	FTT	B	1375	4	-	0/14/14/15	0/0/0/0
4	MYR	B	1376	3	-	0/11/12/13	0/0/0/0
2	LDA	B	1500	-	-	0/13/13/13	0/0/0/0
2	LDA	B	1501	-	-	0/13/13/13	0/0/0/0
2	LDA	C	1344	-	-	0/13/13/13	0/0/0/0
2	LDA	C	1345	-	-	0/13/13/13	0/0/0/0
2	LDA	C	1346	-	-	0/13/13/13	0/0/0/0
2	LDA	C	1347	-	-	0/13/13/13	0/0/0/0
2	LDA	C	1348	-	-	0/8/8/13	0/0/0/0
2	LDA	C	1349	-	-	0/5/5/13	0/0/0/0
2	LDA	C	1350	-	-	0/13/13/13	0/0/0/0
2	LDA	C	1351	-	-	0/13/13/13	0/0/0/0
2	LDA	C	1352	-	-	0/8/8/13	0/0/0/0
2	LDA	C	1353	-	-	0/13/13/13	0/0/0/0
2	LDA	C	1354	-	-	0/8/8/13	0/0/0/0
2	LDA	C	1355	-	-	0/6/6/13	0/0/0/0
2	LDA	C	1356	-	-	0/13/13/13	0/0/0/0
2	LDA	C	1357	-	-	0/13/13/13	0/0/0/0
2	LDA	C	1358	-	-	0/7/7/13	0/0/0/0
2	LDA	C	1359	-	-	0/8/8/13	0/0/0/0
2	LDA	C	1360	-	-	0/13/13/13	0/0/0/0
2	LDA	C	1361	-	-	0/13/13/13	0/0/0/0
2	LDA	C	1362	-	-	0/13/13/13	0/0/0/0
3	FTT	C	1363	4	-	0/14/14/15	0/0/0/0
4	MYR	C	1364	3	-	0/11/12/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FTT	C	1365	4	-	0/14/14/15	0/0/0/0
4	MYR	C	1366	3	-	0/11/12/13	0/0/0/0
3	FTT	C	1367	4	-	0/14/14/15	0/0/0/0
4	MYR	C	1368	3	-	0/11/12/13	0/0/0/0
3	FTT	C	1369	4	-	0/14/14/15	0/0/0/0
4	MYR	C	1370	3	-	0/11/12/13	0/0/0/0
5	SO4	C	1371	-	-	0/0/0/0	0/0/0/0
2	LDA	C	1500	-	-	0/13/13/13	0/0/0/0
2	LDA	C	1501	-	-	0/8/8/13	0/0/0/0
2	LDA	C	1502	-	-	0/5/5/13	0/0/0/0
2	LDA	D	1344	-	-	0/13/13/13	0/0/0/0
2	LDA	D	1345	-	-	0/13/13/13	0/0/0/0
2	LDA	D	1346	-	-	0/13/13/13	0/0/0/0
2	LDA	D	1347	-	-	0/13/13/13	0/0/0/0
2	LDA	D	1348	-	-	0/13/13/13	0/0/0/0
2	LDA	D	1349	-	-	0/13/13/13	0/0/0/0
2	LDA	D	1350	-	-	0/8/8/13	0/0/0/0
2	LDA	D	1351	-	-	0/8/8/13	0/0/0/0
2	LDA	D	1352	-	-	0/13/13/13	0/0/0/0
2	LDA	D	1353	-	-	0/13/13/13	0/0/0/0
2	LDA	D	1354	-	-	0/11/11/13	0/0/0/0
2	LDA	D	1355	-	-	0/13/13/13	0/0/0/0
2	LDA	D	1356	-	-	0/13/13/13	0/0/0/0
2	LDA	D	1357	-	-	0/13/13/13	0/0/0/0
2	LDA	D	1358	-	-	0/5/5/13	0/0/0/0
2	LDA	D	1359	-	-	0/5/5/13	0/0/0/0
2	LDA	D	1360	-	-	0/13/13/13	0/0/0/0
2	LDA	D	1361	-	-	0/5/5/13	0/0/0/0
2	LDA	D	1362	-	-	0/13/13/13	0/0/0/0
2	LDA	D	1363	-	-	0/13/13/13	0/0/0/0
3	FTT	D	1364	4	1/1/1/2	0/14/14/15	0/0/0/0
4	MYR	D	1365	3	-	0/11/12/13	0/0/0/0
5	SO4	D	1366	-	-	0/0/0/0	0/0/0/0
2	LDA	E	1344	-	-	0/13/13/13	0/0/0/0
2	LDA	E	1345	-	-	0/8/8/13	0/0/0/0
2	LDA	E	1346	-	-	0/8/8/13	0/0/0/0
2	LDA	E	1347	-	-	0/8/8/13	0/0/0/0
2	LDA	E	1348	-	-	0/13/13/13	0/0/0/0
2	LDA	E	1349	-	-	0/11/11/13	0/0/0/0
2	LDA	E	1350	-	-	0/13/13/13	0/0/0/0
2	LDA	E	1351	-	-	0/8/8/13	0/0/0/0
2	LDA	E	1352	-	-	0/13/13/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LDA	E	1353	-	-	0/7/7/13	0/0/0/0
2	LDA	E	1354	-	-	0/13/13/13	0/0/0/0
2	LDA	E	1355	-	-	0/13/13/13	0/0/0/0
2	LDA	E	1356	-	-	0/13/13/13	0/0/0/0
2	LDA	E	1357	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1344	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1345	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1346	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1347	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1348	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1349	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1350	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1351	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1352	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1353	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1354	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1355	-	-	0/8/8/13	0/0/0/0
2	LDA	F	1356	-	-	0/8/8/13	0/0/0/0
2	LDA	F	1357	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1358	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1359	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1360	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1361	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1362	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1363	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1364	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1365	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1366	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1500	-	-	0/9/9/13	0/0/0/0
2	LDA	F	1501	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1502	-	-	0/7/7/13	0/0/0/0
2	LDA	F	1503	-	-	0/13/13/13	0/0/0/0
2	LDA	F	1504	-	-	0/13/13/13	0/0/0/0

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1373	LDA	O1-N1	-8.57	1.25	1.42
2	A	1358	LDA	O1-N1	-8.48	1.25	1.42
2	A	1358	LDA	C1-N1	-2.61	1.45	1.51
2	A	1373	LDA	C1-N1	-2.54	1.45	1.51
2	F	1351	LDA	C1-N1	-2.18	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1346	LDA	C1-N1	-2.16	1.46	1.51
3	B	1375	FTT	C2-C3	-2.13	1.50	1.53
2	C	1345	LDA	C1-N1	-2.04	1.46	1.51
2	A	1350[A]	LDA	O1-N1	2.00	1.46	1.42
2	C	1356	LDA	O1-N1	2.01	1.46	1.42
2	F	1365	LDA	O1-N1	2.03	1.46	1.42
2	B	1367	LDA	O1-N1	2.04	1.46	1.42
2	B	1500	LDA	O1-N1	2.04	1.46	1.42
2	F	1346	LDA	O1-N1	2.04	1.46	1.42
2	E	1349	LDA	O1-N1	2.05	1.46	1.42
2	B	1501	LDA	O1-N1	2.06	1.46	1.42
2	C	1353	LDA	O1-N1	2.06	1.46	1.42
2	A	1381	LDA	O1-N1	2.08	1.46	1.42
2	B	1373	LDA	O1-N1	2.08	1.46	1.42
2	D	1360	LDA	O1-N1	2.09	1.46	1.42
2	B	1353	LDA	O1-N1	2.10	1.46	1.42
2	D	1362	LDA	O1-N1	2.10	1.46	1.42
2	A	1348	LDA	O1-N1	2.11	1.46	1.42
2	F	1359	LDA	O1-N1	2.11	1.46	1.42
2	C	1350	LDA	O1-N1	2.12	1.46	1.42
2	F	1503	LDA	O1-N1	2.12	1.46	1.42
2	B	1365	LDA	O1-N1	2.12	1.46	1.42
2	D	1345	LDA	O1-N1	2.13	1.46	1.42
2	C	1349	LDA	O1-N1	2.13	1.46	1.42
2	B	1344	LDA	O1-N1	2.13	1.46	1.42
2	D	1355	LDA	O1-N1	2.13	1.46	1.42
2	B	1345	LDA	O1-N1	2.13	1.46	1.42
2	B	1352	LDA	O1-N1	2.14	1.46	1.42
2	B	1355	LDA	O1-N1	2.14	1.46	1.42
2	E	1348	LDA	O1-N1	2.14	1.46	1.42
2	C	1352	LDA	O1-N1	2.15	1.46	1.42
2	B	1363	LDA	O1-N1	2.15	1.46	1.42
2	C	1346	LDA	O1-N1	2.15	1.46	1.42
2	F	1349	LDA	O1-N1	2.16	1.46	1.42
2	D	1352	LDA	O1-N1	2.16	1.46	1.42
2	A	1369	LDA	O1-N1	2.16	1.46	1.42
2	B	1368	LDA	O1-N1	2.16	1.46	1.42
2	F	1366	LDA	O1-N1	2.16	1.46	1.42
2	C	1351	LDA	O1-N1	2.17	1.46	1.42
2	D	1348	LDA	O1-N1	2.17	1.46	1.42
2	A	1377	LDA	O1-N1	2.17	1.46	1.42
2	C	1345	LDA	O1-N1	2.18	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1361	LDA	O1-N1	2.19	1.46	1.42
2	A	1382	LDA	O1-N1	2.19	1.46	1.42
2	A	1352	LDA	O1-N1	2.20	1.46	1.42
2	C	1344	LDA	O1-N1	2.20	1.46	1.42
2	A	1379	LDA	O1-N1	2.20	1.46	1.42
2	A	1367	LDA	O1-N1	2.21	1.46	1.42
2	E	1346	LDA	O1-N1	2.21	1.46	1.42
2	B	1366	LDA	O1-N1	2.21	1.46	1.42
2	A	1370	LDA	O1-N1	2.21	1.46	1.42
2	A	1344	LDA	O1-N1	2.22	1.46	1.42
2	F	1351	LDA	O1-N1	2.22	1.46	1.42
2	F	1354	LDA	O1-N1	2.23	1.46	1.42
2	F	1345	LDA	O1-N1	2.23	1.46	1.42
2	A	1351	LDA	O1-N1	2.23	1.46	1.42
2	B	1372	LDA	O1-N1	2.23	1.46	1.42
2	E	1345	LDA	O1-N1	2.23	1.46	1.42
2	C	1362	LDA	O1-N1	2.24	1.46	1.42
2	A	1371	LDA	O1-N1	2.25	1.46	1.42
2	D	1356	LDA	O1-N1	2.25	1.46	1.42
2	B	1359	LDA	O1-N1	2.25	1.46	1.42
2	B	1349	LDA	O1-N1	2.25	1.46	1.42
2	C	1361	LDA	O1-N1	2.26	1.46	1.42
2	E	1350	LDA	O1-N1	2.26	1.46	1.42
2	C	1360	LDA	O1-N1	2.27	1.46	1.42
2	B	1370	LDA	O1-N1	2.27	1.46	1.42
2	E	1344	LDA	O1-N1	2.28	1.46	1.42
2	E	1356	LDA	O1-N1	2.28	1.46	1.42
2	D	1346	LDA	O1-N1	2.29	1.46	1.42
2	C	1354	LDA	O1-N1	2.29	1.46	1.42
2	F	1501	LDA	O1-N1	2.30	1.46	1.42
2	F	1362	LDA	O1-N1	2.30	1.46	1.42
2	A	1502	LDA	O1-N1	2.31	1.46	1.42
2	B	1346	LDA	O1-N1	2.31	1.46	1.42
2	B	1354	LDA	O1-N1	2.31	1.46	1.42
2	D	1347	LDA	O1-N1	2.31	1.46	1.42
2	B	1369	LDA	O1-N1	2.32	1.46	1.42
2	B	1364	LDA	O1-N1	2.32	1.46	1.42
2	D	1357	LDA	O1-N1	2.32	1.46	1.42
2	A	1380	LDA	O1-N1	2.32	1.46	1.42
2	C	1355	LDA	O1-N1	2.32	1.46	1.42
2	E	1354	LDA	O1-N1	2.33	1.46	1.42
2	D	1363	LDA	O1-N1	2.33	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1356	LDA	O1-N1	2.33	1.46	1.42
2	A	1349	LDA	O1-N1	2.33	1.46	1.42
2	A	1383	LDA	O1-N1	2.34	1.46	1.42
2	F	1352	LDA	O1-N1	2.34	1.46	1.42
2	F	1353	LDA	O1-N1	2.34	1.46	1.42
2	C	1357	LDA	O1-N1	2.34	1.46	1.42
2	A	1385	LDA	O1-N1	2.34	1.46	1.42
2	A	1355	LDA	O1-N1	2.35	1.46	1.42
2	A	1501	LDA	O1-N1	2.35	1.46	1.42
2	A	1384	LDA	O1-N1	2.35	1.46	1.42
2	F	1358	LDA	O1-N1	2.36	1.46	1.42
2	F	1357	LDA	O1-N1	2.40	1.46	1.42
2	A	1365	LDA	O1-N1	2.41	1.46	1.42
2	A	1353	LDA	O1-N1	2.42	1.46	1.42
2	B	1371	LDA	O1-N1	2.42	1.46	1.42
2	E	1347	LDA	O1-N1	2.44	1.47	1.42
2	A	1357	LDA	O1-N1	2.45	1.47	1.42
2	A	1368	LDA	O1-N1	2.46	1.47	1.42
2	E	1351	LDA	O1-N1	2.46	1.47	1.42
2	D	1353	LDA	O1-N1	2.47	1.47	1.42
2	F	1350	LDA	O1-N1	2.48	1.47	1.42
2	A	1376	LDA	O1-N1	2.48	1.47	1.42
2	F	1361	LDA	O1-N1	2.49	1.47	1.42
2	D	1351	LDA	O1-N1	2.50	1.47	1.42
2	A	1362	LDA	O1-N1	2.52	1.47	1.42
2	F	1360	LDA	O1-N1	2.52	1.47	1.42
2	E	1355	LDA	O1-N1	2.52	1.47	1.42
2	A	1386	LDA	O1-N1	2.52	1.47	1.42
2	B	1350	LDA	O1-N1	2.53	1.47	1.42
2	F	1363	LDA	O1-N1	2.58	1.47	1.42
2	C	1347	LDA	O1-N1	2.58	1.47	1.42
2	C	1359	LDA	O1-N1	2.59	1.47	1.42
2	B	1374	LDA	O1-N1	2.60	1.47	1.42
2	F	1500	LDA	O1-N1	2.61	1.47	1.42
2	A	1388	LDA	O1-N1	2.64	1.47	1.42
2	C	1348	LDA	O1-N1	2.65	1.47	1.42
2	A	1350[B]	LDA	O1-N1	2.69	1.47	1.42
2	B	1360	LDA	O1-N1	2.71	1.47	1.42
2	E	1357	LDA	O1-N1	2.77	1.47	1.42
2	D	1350	LDA	O1-N1	2.83	1.47	1.42
2	E	1352	LDA	O1-N1	3.11	1.48	1.42
3	C	1365	FTT	O2-C1	3.21	1.39	1.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1364	FTT	O2-C1	3.21	1.39	1.19
3	C	1367	FTT	O2-C1	3.24	1.39	1.19
3	C	1369	FTT	O2-C1	3.24	1.39	1.19
3	B	1375	FTT	O2-C1	3.25	1.39	1.19
3	C	1363	FTT	O2-C1	3.27	1.39	1.19

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1504	LDA	O1-N1-C1	-10.82	82.72	109.27
2	C	1347	LDA	O1-N1-C1	-8.79	87.70	109.27
2	A	1387	LDA	CM2-N1-CM1	-3.80	103.71	110.99
2	D	1362	LDA	CM2-N1-CM1	-3.28	104.72	110.99
2	A	1360	LDA	CM2-N1-CM1	-3.27	104.74	110.99
2	F	1504	LDA	C8-C7-C6	-3.21	97.92	114.45
2	A	1368	LDA	CM2-N1-CM1	-3.12	105.03	110.99
2	B	1371	LDA	CM2-N1-CM1	-3.08	105.10	110.99
2	A	1360	LDA	CM1-N1-C1	-3.04	103.84	110.23
2	B	1366	LDA	C4-C3-C2	-2.78	100.11	114.45
2	D	1347	LDA	C7-C6-C5	-2.78	100.12	114.45
2	B	1366	LDA	CM1-N1-C1	-2.77	104.42	110.23
2	F	1364	LDA	CM2-N1-CM1	-2.77	105.69	110.99
2	D	1354	LDA	CM2-N1-CM1	-2.60	106.01	110.99
2	A	1357	LDA	CM2-N1-CM1	-2.56	106.09	110.99
2	A	1387	LDA	CM1-N1-C1	-2.53	104.92	110.23
3	B	1375	FTT	O2-C1-C2	-2.48	117.47	125.48
3	D	1364	FTT	O2-C1-C2	-2.47	117.48	125.48
2	A	1367	LDA	CM2-N1-CM1	-2.46	106.27	110.99
2	B	1348	LDA	C8-C7-C6	-2.41	102.05	114.45
2	F	1351	LDA	C9-C8-C7	-2.41	102.06	114.45
2	D	1347	LDA	C5-C4-C3	-2.40	102.07	114.45
2	A	1345	LDA	CM2-N1-C1	-2.38	105.24	110.23
3	C	1365	FTT	O2-C1-C2	-2.37	117.82	125.48
3	C	1369	FTT	O2-C1-C2	-2.36	117.82	125.48
2	A	1346	LDA	C5-C4-C3	-2.36	102.29	114.45
2	B	1371	LDA	CM1-N1-C1	-2.36	105.28	110.23
2	D	1363	LDA	C7-C6-C5	-2.35	102.33	114.45
3	C	1367	FTT	O2-C1-C2	-2.29	118.07	125.48
2	A	1368	LDA	CM2-N1-C1	-2.24	105.53	110.23
2	D	1353	LDA	C9-C8-C7	-2.22	103.01	114.45
2	A	1388	LDA	C7-C6-C5	-2.20	103.11	114.45
3	C	1363	FTT	O2-C1-C2	-2.20	118.37	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1366	LDA	CM2-N1-CM1	-2.20	106.79	110.99
2	B	1366	LDA	CM2-N1-CM1	-2.19	106.81	110.99
2	A	1370	LDA	C9-C8-C7	-2.16	103.30	114.45
2	B	1353	LDA	C9-C8-C7	-2.15	103.37	114.45
2	B	1371	LDA	C10-C9-C8	-2.14	103.42	114.45
2	A	1361	LDA	C6-C5-C4	-2.14	103.44	114.45
2	A	1346	LDA	C8-C7-C6	-2.13	103.46	114.45
2	B	1351	LDA	C6-C5-C4	-2.12	103.51	114.45
2	F	1500	LDA	CM2-N1-CM1	-2.11	106.96	110.99
2	D	1353	LDA	C7-C6-C5	-2.10	103.63	114.45
2	F	1365	LDA	C4-C3-C2	-2.07	103.78	114.45
2	D	1360	LDA	C8-C7-C6	-2.06	103.81	114.45
2	B	1374	LDA	C6-C5-C4	-2.06	103.83	114.45
2	D	1354	LDA	CM2-N1-C1	-2.04	105.94	110.23
2	D	1363	LDA	C4-C3-C2	-2.03	103.99	114.45
2	C	1501	LDA	C5-C4-C3	-2.01	104.11	114.45
2	F	1504	LDA	C10-C9-C8	-2.00	104.14	114.45
2	F	1344	LDA	C1-C2-C3	2.01	119.13	110.67
2	C	1355	LDA	CM2-N1-C1	2.07	114.58	110.23
3	D	1364	FTT	C3-C2-C1	2.08	116.79	112.24
2	C	1354	LDA	C1-C2-C3	2.12	119.58	110.67
2	F	1504	LDA	CM2-N1-C1	2.16	114.77	110.23
2	B	1369	LDA	CM2-N1-C1	2.19	114.83	110.23
3	C	1365	FTT	C3-C2-C1	2.26	117.18	112.24
2	A	1351	LDA	CM2-N1-C1	2.30	115.06	110.23
2	B	1366	LDA	CM2-N1-C1	2.30	115.07	110.23
4	D	1365	MYR	C3-C2-C1	2.39	119.60	113.05
2	F	1504	LDA	C7-C6-C5	2.42	126.93	114.45
2	A	1355	LDA	CM1-N1-C1	2.42	115.33	110.23
3	C	1369	FTT	C3-C2-C1	2.62	117.97	112.24
3	C	1367	FTT	C3-C2-C1	2.62	117.97	112.24
3	C	1363	FTT	C3-C2-C1	2.65	118.05	112.24
4	B	1376	MYR	C3-C2-C1	2.72	120.50	113.05
2	B	1366	LDA	C1-C2-C3	2.94	123.02	110.67
2	F	1504	LDA	C6-C5-C4	3.02	130.02	114.45
2	D	1354	LDA	CM1-N1-C1	3.02	116.58	110.23
2	A	1360	LDA	CM2-N1-C1	3.11	116.78	110.23
2	A	1368	LDA	CM1-N1-C1	3.18	116.92	110.23
2	B	1371	LDA	CM2-N1-C1	3.19	116.93	110.23
2	A	1387	LDA	CM2-N1-C1	3.28	117.13	110.23
2	E	1347	LDA	CM2-N1-C1	3.50	117.59	110.23
2	F	1504	LDA	CM2-N1-CM1	3.74	118.14	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1362	LDA	CM1-N1-C1	3.93	118.48	110.23
2	C	1347	LDA	CM1-N1-C1	4.04	118.72	110.23
2	B	1372	LDA	CM1-N1-C1	4.09	118.83	110.23
2	C	1347	LDA	CM2-N1-C1	4.22	119.10	110.23
2	C	1347	LDA	CM2-N1-CM1	4.84	120.25	110.99
2	F	1504	LDA	CM1-N1-C1	6.34	123.56	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	1364	FTT	C3

There are no torsion outliers.

There are no ring outliers.

138 monomers are involved in 239 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1346	LDA	3	0
2	A	1347	LDA	1	0
2	A	1348	LDA	3	0
2	A	1349	LDA	1	0
2	A	1350[B]	LDA	9	0
2	A	1351	LDA	2	0
2	A	1353	LDA	1	0
2	A	1354	LDA	9	0
2	A	1355	LDA	4	0
2	A	1356	LDA	1	0
2	A	1357	LDA	7	0
2	A	1358	LDA	3	0
2	A	1359	LDA	1	0
2	A	1362	LDA	1	0
2	A	1365	LDA	1	0
2	A	1366	LDA	3	0
2	A	1367	LDA	3	0
2	A	1368	LDA	4	0
2	A	1369	LDA	2	0
2	A	1370	LDA	2	0
2	A	1371	LDA	1	0
2	A	1372	LDA	2	0
2	A	1373	LDA	3	0
2	A	1374	LDA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1375	LDA	3	0
2	A	1376	LDA	2	0
2	A	1377	LDA	1	0
2	A	1379	LDA	5	0
2	A	1380	LDA	3	0
2	A	1382	LDA	2	0
2	A	1383	LDA	5	0
2	A	1384	LDA	3	0
2	A	1385	LDA	4	0
2	A	1386	LDA	4	0
2	A	1387	LDA	9	0
2	A	1388	LDA	6	0
2	A	1502	LDA	3	0
2	B	1344	LDA	1	0
2	B	1345	LDA	4	0
2	B	1347	LDA	2	0
2	B	1348	LDA	3	0
2	B	1349	LDA	1	0
2	B	1350	LDA	1	0
2	B	1351	LDA	2	0
2	B	1353	LDA	2	0
2	B	1354	LDA	2	0
2	B	1355	LDA	1	0
2	B	1356	LDA	1	0
2	B	1359	LDA	2	0
2	B	1360	LDA	2	0
2	B	1361	LDA	1	0
2	B	1362	LDA	1	0
2	B	1363	LDA	3	0
2	B	1365	LDA	2	0
2	B	1366	LDA	5	0
2	B	1367	LDA	2	0
2	B	1368	LDA	1	0
2	B	1369	LDA	1	0
2	B	1371	LDA	6	0
2	B	1372	LDA	5	0
2	B	1373	LDA	6	0
2	B	1374	LDA	3	0
2	B	1500	LDA	1	0
2	B	1501	LDA	3	0
2	C	1344	LDA	1	0
2	C	1345	LDA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1346	LDA	1	0
2	C	1347	LDA	3	0
2	C	1351	LDA	3	0
2	C	1352	LDA	6	0
2	C	1353	LDA	2	0
2	C	1354	LDA	1	0
2	C	1355	LDA	2	0
2	C	1357	LDA	1	0
2	C	1358	LDA	1	0
2	C	1359	LDA	1	0
2	C	1360	LDA	4	0
2	C	1361	LDA	2	0
4	C	1364	MYR	1	0
3	C	1365	FTT	4	0
4	C	1366	MYR	2	0
3	C	1367	FTT	1	0
4	C	1368	MYR	1	0
3	C	1369	FTT	3	0
4	C	1370	MYR	2	0
2	C	1500	LDA	2	0
2	C	1501	LDA	5	0
2	D	1344	LDA	3	0
2	D	1345	LDA	2	0
2	D	1346	LDA	5	0
2	D	1347	LDA	1	0
2	D	1348	LDA	1	0
2	D	1350	LDA	1	0
2	D	1352	LDA	3	0
2	D	1353	LDA	1	0
2	D	1354	LDA	4	0
2	D	1355	LDA	2	0
2	D	1356	LDA	5	0
2	D	1357	LDA	5	0
2	D	1360	LDA	1	0
2	D	1362	LDA	3	0
2	E	1344	LDA	3	0
2	E	1345	LDA	1	0
2	E	1346	LDA	2	0
2	E	1347	LDA	2	0
2	E	1348	LDA	1	0
2	E	1349	LDA	1	0
2	E	1352	LDA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1354	LDA	2	0
2	E	1355	LDA	1	0
2	E	1356	LDA	3	0
2	E	1357	LDA	3	0
2	F	1344	LDA	6	0
2	F	1345	LDA	1	0
2	F	1346	LDA	4	0
2	F	1347	LDA	3	0
2	F	1348	LDA	3	0
2	F	1349	LDA	2	0
2	F	1350	LDA	1	0
2	F	1351	LDA	6	0
2	F	1352	LDA	6	0
2	F	1353	LDA	1	0
2	F	1354	LDA	1	0
2	F	1355	LDA	3	0
2	F	1356	LDA	1	0
2	F	1357	LDA	2	0
2	F	1358	LDA	6	0
2	F	1359	LDA	4	0
2	F	1360	LDA	3	0
2	F	1362	LDA	6	0
2	F	1363	LDA	1	0
2	F	1364	LDA	2	0
2	F	1365	LDA	5	0
2	F	1366	LDA	4	0
2	F	1500	LDA	2	0
2	F	1501	LDA	2	0
2	F	1502	LDA	1	0
2	F	1504	LDA	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	153:GLY	C	154:LYS	N	1.08

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	343/343 (100%)	-0.55	5 (1%) 74 72	20, 30, 60, 117	1 (0%)
1	B	343/343 (100%)	-0.48	5 (1%) 74 72	21, 30, 61, 117	0
1	C	343/343 (100%)	-0.50	9 (2%) 56 54	21, 31, 62, 117	1 (0%)
1	D	343/343 (100%)	-0.48	6 (1%) 70 68	19, 30, 61, 117	1 (0%)
1	E	343/343 (100%)	-0.55	6 (1%) 70 68	21, 30, 62, 117	0
1	F	343/343 (100%)	-0.57	5 (1%) 74 72	20, 31, 62, 117	0
All	All	2058/2058 (100%)	-0.52	36 (1%) 70 68	19, 31, 62, 117	3 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	141	TYR	8.7
1	B	141	TYR	7.2
1	C	139	PHE	5.9
1	B	7	ASP	5.3
1	E	141	TYR	4.2
1	B	6	LYS	3.8
1	F	141	TYR	3.7
1	C	140	GLY	3.7
1	D	7	ASP	3.7
1	D	6	LYS	3.6
1	C	8	GLY	3.4
1	E	6	LYS	3.2
1	C	7	ASP	3.2
1	F	8	GLY	3.0
1	B	139	PHE	3.0
1	C	6	LYS	2.9
1	C	138	GLY	2.7
1	E	143	ASP	2.7
1	E	7	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	140	GLY	2.7
1	A	7	ASP	2.6
1	E	139	PHE	2.4
1	D	5	ASN	2.4
1	A	6	LYS	2.3
1	A	5	ASN	2.3
1	F	6	LYS	2.3
1	D	50[A]	GLN	2.3
1	B	8	GLY	2.2
1	F	266	ASP	2.2
1	A	4	TYR	2.2
1	C	50[A]	GLN	2.2
1	D	4	TYR	2.1
1	F	7	ASP	2.1
1	A	8	GLY	2.1
1	D	8	GLY	2.0
1	C	142	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	LDA	E	1345	11/16	0.61	0.59	49.94	39,91,104,109	0
2	LDA	F	1365	16/16	0.49	0.45	44.07	73,91,118,125	0
4	MYR	C	1364	15/16	0.80	0.30	34.56	55,76,105,109	0
2	LDA	A	1383	16/16	0.78	0.49	30.96	62,79,118,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LDA	E	1349	14/16	0.83	0.44	30.60	51,72,94,110	0
2	LDA	B	1344	10/16	0.81	0.30	30.04	49,59,83,92	0
2	LDA	F	1357	16/16	0.66	0.51	24.43	68,115,133,133	0
2	LDA	A	1360	12/16	0.88	0.38	19.92	72,84,95,96	0
3	FTT	C	1363	16/17	0.80	0.28	18.58	43,63,98,108	0
2	LDA	A	1353	11/16	0.84	0.35	18.49	43,57,101,108	0
2	LDA	F	1354	16/16	0.79	0.30	15.99	41,85,92,93	0
2	LDA	C	1351	16/16	0.81	0.34	15.57	58,70,106,110	0
2	LDA	D	1350	11/16	0.76	0.35	15.44	40,53,95,106	0
2	LDA	F	1351	16/16	0.75	0.43	15.23	84,90,97,102	0
2	LDA	F	1359	16/16	0.53	0.48	15.22	85,103,115,119	0
2	LDA	D	1353	16/16	0.69	0.44	14.97	51,83,118,120	0
2	LDA	D	1345	16/16	0.69	0.41	12.84	46,77,123,135	0
2	LDA	A	1373	16/16	0.76	0.27	12.30	43,64,116,117	0
2	LDA	F	1345	16/16	0.77	0.27	12.24	33,55,108,110	0
2	LDA	D	1352	16/16	0.80	0.30	12.23	54,79,81,83	0
2	LDA	B	1360	16/16	0.73	0.25	12.12	45,58,114,115	0
2	LDA	B	1364	16/16	0.70	0.27	11.91	41,75,85,93	0
2	LDA	A	1387	16/16	0.67	0.32	11.52	74,93,117,121	0
2	LDA	A	1501	11/16	0.66	0.36	11.50	35,82,91,94	0
2	LDA	D	1347	16/16	0.69	0.31	11.29	32,80,116,119	0
2	LDA	F	1355	11/16	0.66	0.45	11.29	51,73,111,116	0
2	LDA	B	1363	16/16	0.67	0.44	11.28	57,82,116,117	0
2	LDA	A	1364	9/16	0.79	0.33	11.00	46,58,84,86	0
2	LDA	E	1348	16/16	0.78	0.32	10.46	57,68,89,91	0
2	LDA	F	1344	16/16	0.48	0.47	9.90	30,83,124,129	0
2	LDA	C	1344	16/16	0.47	0.55	9.76	48,99,125,129	0
2	LDA	B	1365	16/16	0.73	0.43	9.72	56,88,105,110	0
2	LDA	A	1376	16/16	0.85	0.27	9.44	30,76,102,109	0
2	LDA	E	1353	10/16	0.65	0.35	9.41	37,66,79,83	0
2	LDA	A	1500	11/16	0.82	0.25	9.36	31,62,72,74	0
2	LDA	A	1361	16/16	0.73	0.41	9.34	63,76,83,87	0
2	LDA	A	1362	16/16	0.51	0.49	9.26	46,89,110,113	0
2	LDA	B	1345	16/16	0.82	0.37	9.01	60,71,83,87	0
2	LDA	F	1346	16/16	0.86	0.18	8.95	52,58,84,90	0
2	LDA	A	1359	8/16	0.90	0.27	8.82	35,41,72,78	0
2	LDA	D	1344	16/16	0.75	0.40	8.69	48,76,87,91	0
2	LDA	F	1352	16/16	0.58	0.51	8.54	54,90,134,142	0
2	LDA	A	1369	16/16	0.67	0.24	8.53	52,63,112,114	0
2	LDA	B	1359	16/16	0.81	0.23	8.48	37,62,94,94	0
2	LDA	A	1354	16/16	0.84	0.23	8.42	39,50,109,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LDA	A	1352	12/16	0.77	0.49	8.32	70,79,112,114	0
2	LDA	C	1358	10/16	0.90	0.21	8.31	36,44,70,71	0
2	LDA	C	1362	16/16	0.72	0.40	8.26	82,90,123,125	0
2	LDA	B	1358	12/16	0.75	0.28	8.08	56,70,98,107	0
2	LDA	E	1357	16/16	0.62	0.60	7.99	88,108,137,137	0
2	LDA	D	1361	8/16	0.93	0.25	7.69	49,59,91,93	0
2	LDA	E	1352	16/16	0.81	0.32	7.56	44,68,77,83	0
2	LDA	A	1379	16/16	0.74	0.24	7.44	43,57,117,122	0
2	LDA	C	1348	11/16	0.69	0.40	7.33	47,63,112,129	0
2	LDA	E	1344	16/16	0.77	0.28	6.77	37,67,112,124	0
2	LDA	F	1347	16/16	0.81	0.24	6.66	46,64,100,107	0
2	LDA	C	1356	16/16	0.85	0.29	6.61	70,78,81,81	0
2	LDA	A	1366	16/16	0.74	0.34	6.36	51,77,94,112	0
2	LDA	A	1357	16/16	0.77	0.26	6.26	45,58,106,106	0
2	LDA	D	1348	16/16	0.74	0.39	6.13	66,76,105,106	0
2	LDA	F	1361	16/16	0.49	0.40	6.07	64,89,122,124	0
2	LDA	B	1350	16/16	0.77	0.20	6.07	36,54,99,110	0
2	LDA	A	1372	16/16	0.83	0.26	5.76	40,61,87,87	0
2	LDA	B	1500	16/16	0.90	0.20	5.60	42,51,70,73	0
3	FTT	B	1375	16/17	0.81	0.20	5.49	25,35,70,73	0
2	LDA	C	1357	16/16	0.67	0.34	5.40	52,74,114,114	0
2	LDA	B	1347	16/16	0.83	0.21	5.33	43,54,96,106	0
4	MYR	B	1376	15/16	0.81	0.23	5.29	30,41,74,77	0
2	LDA	F	1349	16/16	0.75	0.26	5.20	36,54,93,118	0
2	LDA	C	1353	16/16	0.74	0.26	5.20	50,65,101,116	0
4	MYR	C	1366	15/16	0.80	0.20	5.15	56,65,91,92	0
2	LDA	A	1370	16/16	0.78	0.22	4.98	35,45,97,100	0
2	LDA	E	1356	16/16	0.69	0.41	4.97	72,81,109,114	0
2	LDA	B	1352	16/16	0.79	0.21	4.87	47,62,90,104	0
2	LDA	A	1371	16/16	0.85	0.24	4.83	40,72,99,100	0
2	LDA	F	1353	16/16	0.66	0.39	4.81	67,82,122,127	0
2	LDA	B	1501	16/16	0.82	0.21	4.81	34,45,102,113	0
2	LDA	F	1350	16/16	0.79	0.28	4.70	45,68,86,100	0
2	LDA	B	1354	16/16	0.82	0.28	4.46	50,71,96,98	0
2	LDA	C	1345	16/16	0.83	0.22	4.31	33,59,93,100	0
2	LDA	B	1353	16/16	0.86	0.20	4.24	30,43,87,94	0
2	LDA	B	1348	16/16	0.85	0.25	4.07	39,56,98,112	0
2	LDA	C	1346	16/16	0.85	0.23	3.92	30,63,89,90	0
2	LDA	A	1348	16/16	0.80	0.23	3.90	43,56,99,101	0
2	LDA	F	1348	16/16	0.73	0.23	3.85	42,53,101,119	0
3	FTT	D	1364	16/17	0.57	0.51	3.82	45,83,119,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	LDA	A	1365	16/16	0.85	0.36	3.41	69,81,88,92	0
2	LDA	A	1344	16/16	0.84	0.23	2.84	38,56,88,90	0
2	LDA	A	1345	16/16	0.91	0.17	2.78	21,37,55,65	0
2	LDA	A	1346	16/16	0.92	0.17	2.02	27,40,58,76	0
2	LDA	A	1347	16/16	0.87	0.16	1.95	33,43,57,64	0
2	LDA	C	1347	16/16	0.89	0.14	1.90	40,49,77,87	0
2	LDA	B	1346	16/16	0.87	0.14	1.35	34,42,71,75	0
2	LDA	F	1501	16/16	0.59	0.38	0.93	68,96,121,124	0
2	LDA	B	1351	16/16	0.81	0.18	0.89	42,55,88,94	0
2	LDA	F	1500	12/16	0.81	0.23	-	43,55,95,97	0
2	LDA	A	1388	16/16	0.52	0.41	-	106,120,151,152	0
2	LDA	A	1378	9/16	0.93	0.18	-	56,59,94,104	0
2	LDA	D	1360	16/16	0.78	0.45	-	74,107,130,131	0
2	LDA	D	1362	16/16	0.52	0.40	-	73,125,132,135	0
2	LDA	D	1357	16/16	0.68	0.61	-	104,124,138,139	0
2	LDA	B	1355	16/16	0.76	0.28	-	51,60,109,117	0
2	LDA	A	1351	14/16	0.68	0.66	-	98,105,111,111	0
3	FTT	C	1367	16/17	0.44	0.51	-	78,113,121,130	0
2	LDA	B	1366	16/16	0.67	0.40	-	76,86,109,118	0
2	LDA	C	1500	16/16	0.52	0.55	-	96,108,118,123	0
2	LDA	A	1363	9/16	0.83	0.44	-	67,74,83,86	0
2	LDA	D	1351	11/16	0.71	0.60	-	78,94,113,116	0
2	LDA	D	1358	8/16	0.71	0.74	-	116,121,132,134	0
2	LDA	C	1355	9/16	0.87	0.30	-	91,105,108,114	0
2	LDA	C	1360	16/16	0.77	0.47	-	77,102,123,124	0
2	LDA	A	1356	11/16	0.82	0.40	-	78,84,104,107	0
2	LDA	A	1384	16/16	0.58	0.53	-	90,98,135,141	0
4	MYR	C	1368	15/16	0.49	0.56	-	116,122,132,135	0
2	LDA	F	1502	10/16	0.69	0.32	-	73,82,91,94	0
2	LDA	C	1354	11/16	0.65	0.42	-	87,100,119,119	0
2	LDA	A	1381	16/16	0.49	0.49	-	75,98,119,122	0
2	LDA	E	1354	16/16	0.42	0.41	-	109,115,121,129	0
2	LDA	A	1375	9/16	0.76	0.38	-	95,102,106,107	0
2	LDA	A	1367	16/16	0.85	0.17	-	46,57,79,87	0
2	LDA	A	1350[A]	16/16	0.70	0.36	-	53,70,76,81	16
2	LDA	F	1503	16/16	0.58	0.43	-	83,101,126,130	0
2	LDA	A	1385	16/16	0.76	0.29	-	43,80,129,131	0
2	LDA	D	1349	16/16	0.35	0.72	-	105,124,152,155	0
2	LDA	D	1356	16/16	0.67	0.58	-	63,86,131,131	0
2	LDA	E	1355	16/16	0.74	0.27	-	54,65,130,131	0
2	LDA	B	1362	9/16	0.79	0.36	-	80,82,85,86	0
2	LDA	F	1362	16/16	0.27	0.62	-	117,125,146,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LDA	F	1360	16/16	0.46	0.53	-	97,109,121,127	0
2	LDA	C	1352	11/16	0.75	0.27	-	58,65,102,107	0
2	LDA	A	1368	16/16	0.77	0.22	-	46,62,132,135	0
2	LDA	D	1363	16/16	0.64	0.36	-	79,103,116,122	0
2	LDA	B	1369	16/16	0.78	0.46	-	60,67,125,130	0
2	LDA	E	1351	11/16	0.55	0.43	-	66,83,123,129	0
2	LDA	A	1355	16/16	0.71	0.33	-	63,94,124,126	0
3	FTT	C	1365	16/17	0.70	0.37	-	82,93,98,98	0
2	LDA	B	1349	13/16	0.76	0.24	-	42,60,94,97	0
2	LDA	C	1350	16/16	0.65	0.55	-	73,93,106,107	0
2	LDA	C	1361	16/16	0.79	0.44	-	55,95,110,111	0
2	LDA	A	1350[B]	16/16	0.70	0.36	-	26,67,75,75	16
2	LDA	C	1501	11/16	0.74	0.28	-	48,59,97,101	0
4	MYR	D	1365	15/16	0.43	0.40	-	63,79,126,126	0
2	LDA	C	1349	8/16	0.69	0.65	-	84,104,111,118	0
2	LDA	B	1374	16/16	0.60	0.29	-	46,89,128,128	0
2	LDA	A	1358	16/16	0.78	0.24	-	48,62,104,109	0
2	LDA	A	1386	16/16	0.67	0.29	-	63,79,129,131	0
2	LDA	D	1355	16/16	0.59	0.43	-	109,122,131,139	0
2	LDA	C	1359	11/16	0.66	0.42	-	75,93,112,120	0
2	LDA	C	1502	8/16	0.70	0.24	-	73,78,81,81	0
2	LDA	A	1377	16/16	0.64	0.38	-	70,88,124,131	0
2	LDA	B	1372	16/16	0.59	0.51	-	85,110,151,152	0
2	LDA	D	1359	8/16	0.71	0.46	-	74,99,104,105	0
5	SO4	C	1371	5/5	0.92	0.30	-	88,97,101,105	0
2	LDA	B	1370	8/16	0.79	0.29	-	60,78,91,95	0
2	LDA	E	1350	16/16	0.73	0.39	-	55,81,113,118	0
2	LDA	D	1354	14/16	0.67	0.49	-	77,95,116,121	0
2	LDA	A	1374	8/16	0.94	0.17	-	68,74,82,89	0
2	LDA	B	1367	16/16	0.83	0.50	-	75,81,110,111	0
2	LDA	F	1364	16/16	0.59	0.61	-	79,99,131,135	0
2	LDA	A	1502	11/16	0.56	0.59	-	60,88,128,131	0
2	LDA	F	1356	11/16	0.64	0.58	-	93,96,113,116	0
2	LDA	A	1380	11/16	0.61	0.35	-	85,112,131,131	0
2	LDA	B	1357	9/16	0.88	0.15	-	48,51,77,82	0
2	LDA	B	1373	16/16	0.61	0.33	-	97,111,121,123	0
2	LDA	F	1363	16/16	0.45	0.56	-	105,119,140,141	0
2	LDA	B	1356	16/16	0.77	0.38	-	73,81,104,105	0
2	LDA	D	1346	16/16	0.61	0.42	-	62,94,128,129	0
2	LDA	B	1361	9/16	0.65	0.40	-	57,76,86,86	0
2	LDA	F	1504	16/16	0.76	0.29	-	57,79,105,109	0
2	LDA	E	1346	11/16	0.52	0.54	-	50,92,101,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LDA	F	1366	16/16	0.64	0.40	-	75,99,115,123	0
2	LDA	A	1349	16/16	0.53	0.37	-	59,109,130,134	0
2	LDA	B	1368	11/16	0.73	0.54	-	74,87,111,115	0
4	MYR	C	1370	15/16	0.66	0.40	-	90,99,122,124	0
2	LDA	A	1382	16/16	0.75	0.35	-	78,99,129,133	0
5	SO4	D	1366	5/5	0.94	0.23	-	82,93,95,98	0
2	LDA	B	1371	16/16	0.71	0.45	-	79,93,126,129	0
2	LDA	E	1347	11/16	0.78	0.35	-	62,128,148,148	0
2	LDA	F	1358	16/16	0.55	0.54	-	102,109,143,145	0
3	FTT	C	1369	16/17	0.66	0.29	-	74,99,122,124	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.