



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:17 PM UTC

PDB ID : 2IWV / pdb_00002iww
Title : Structure of the monomeric outer membrane porin OmpG in the open and closed conformation
Authors : Yildiz, O.; Vinothkumar, K.R.; Goswami, P.; Kuehlbrandt, W.
Deposited on : 2006-07-04
Resolution : 2.30 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

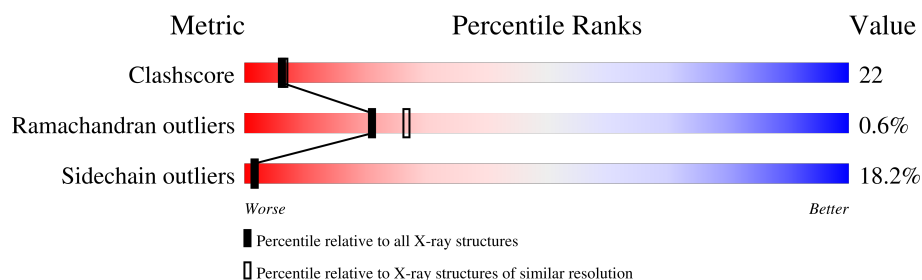
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	281	
1	B	281	
1	C	281	
1	D	281	

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
3	LDA	A	1313	-	-	X	-
3	LDA	A	1315	-	-	X	-
3	LDA	A	1318	-	-	X	-
3	LDA	A	1319	-	-	X	-
3	LDA	A	413	-	-	X	-
3	LDA	B	1292	-	-	X	-
3	LDA	C	1291	-	-	X	-
3	LDA	D	1301	-	-	X	-
3	LDA	D	1307	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12128 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.

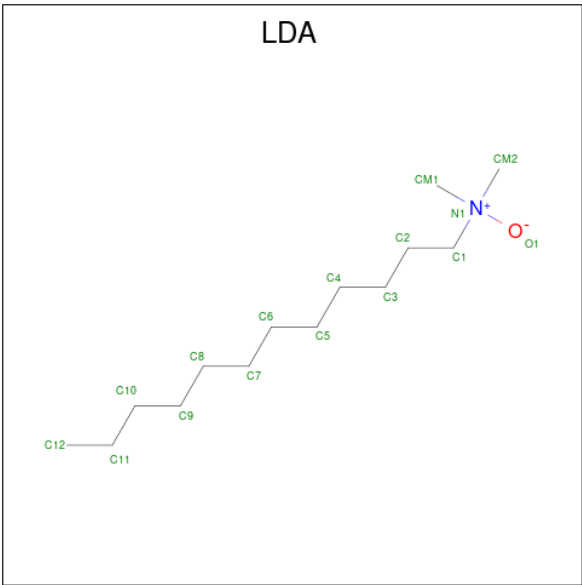
- Molecule 1 is a protein called OUTER MEMBRANE PROTEIN G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2298	1461	381	451	5			
1	B	277	Total	C	N	O	S	0	0	0
			2298	1461	381	451	5			
1	C	277	Total	C	N	O	S	0	0	0
			2298	1461	381	451	5			
1	D	277	Total	C	N	O	S	0	0	0
			2298	1461	381	451	5			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	Ca	0	0
			9	9		
2	B	9	Total	Ca	0	0
			9	9		
2	C	8	Total	Ca	0	0
			8	8		
2	D	7	Total	Ca	0	0
			7	7		

- Molecule 3 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		

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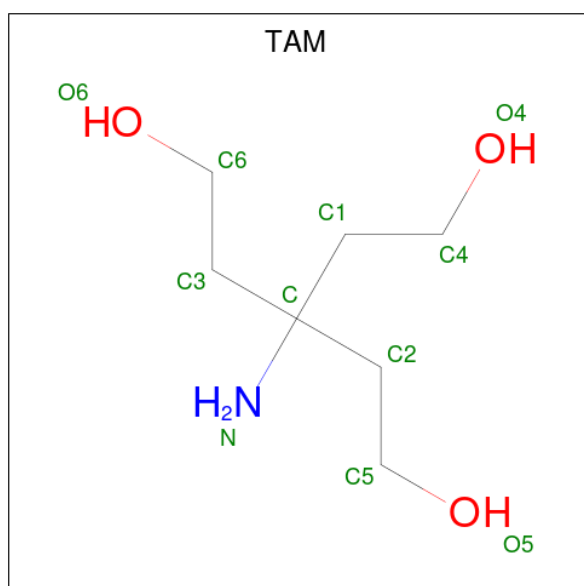
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	C	1	Total	C	N	O	0	0
			16	14	1	1		
3	D	1	Total	C	N	O	0	0
			16	14	1	1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

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

- Molecule 4 is TRIS(HYDROXYETHYL)AMINOMETHANE (CCD ID: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 5 is water.

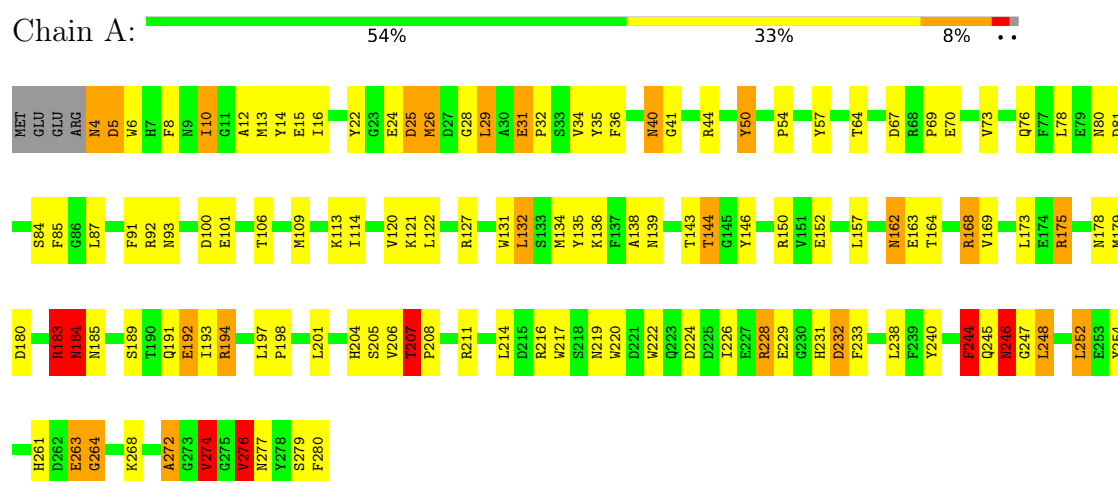
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	110	Total	O	0	0
			110	110		
5	B	124	Total	O	0	0
			124	124		
5	C	112	Total	O	0	0
			112	112		
5	D	114	Total	O	0	0
			114	114		

3 Residue-property plots

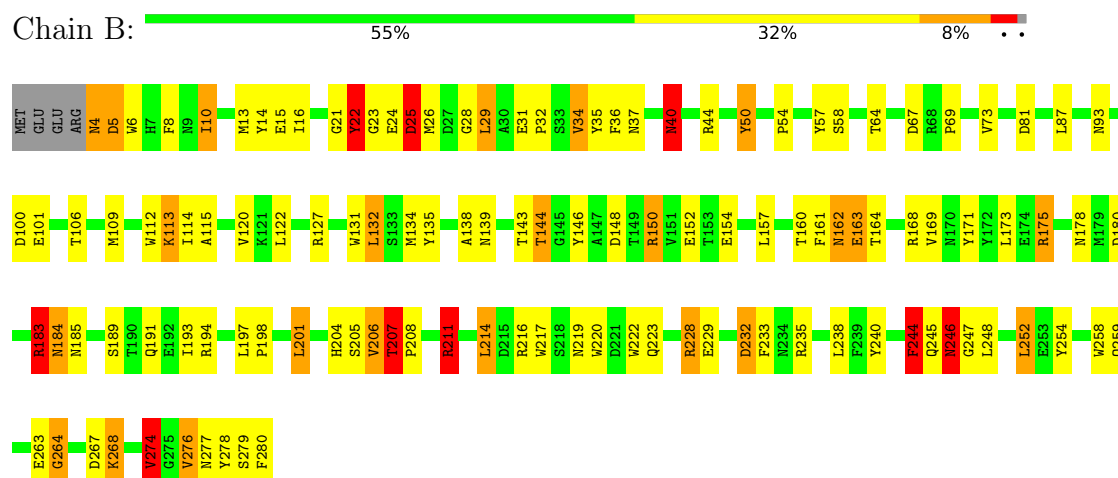
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: OUTER MEMBRANE PROTEIN G

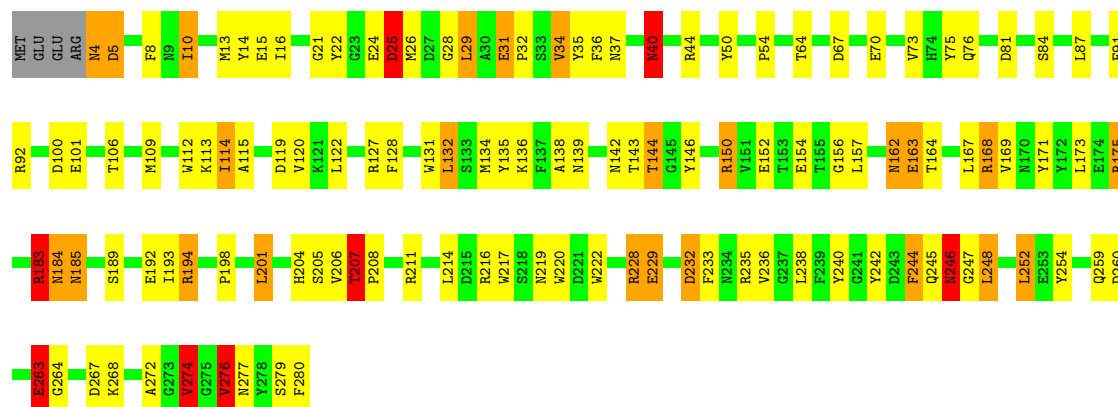


• Molecule 1: OUTER MEMBRANE PROTEIN G



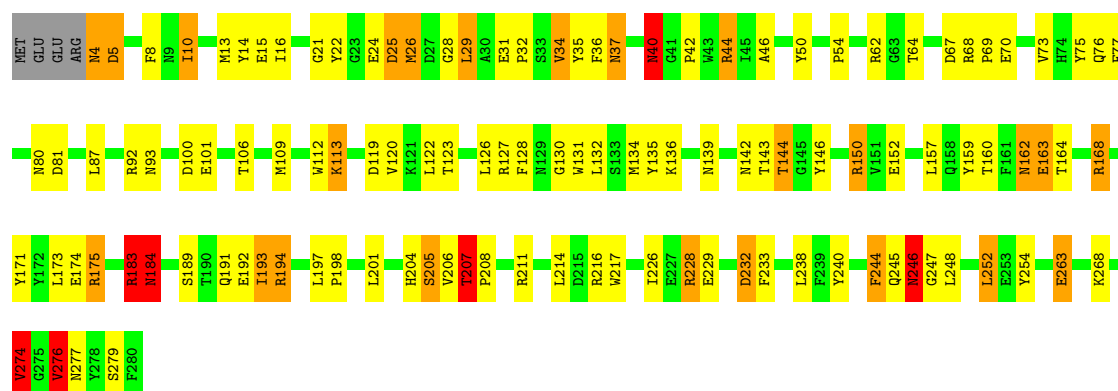
• Molecule 1: OUTER MEMBRANE PROTEIN G





• Molecule 1: OUTER MEMBRANE PROTEIN G

Chain D: 57% 31% 9% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.60 Å 77.00 Å 103.90 Å 79.30° 73.40° 74.30°	Depositor
Resolution (Å)	14.98 – 2.30	Depositor
% Data completeness (in resolution range)	100.0 (14.98-2.30)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.224 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12128	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, LDA, TAM

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	1.16	1/2372 (0.0%)	1.28	21/3226 (0.7%)
1	B	1.21	6/2372 (0.3%)	1.32	28/3226 (0.9%)
1	C	1.21	2/2372 (0.1%)	1.29	27/3226 (0.8%)
1	D	1.18	5/2372 (0.2%)	1.30	21/3226 (0.7%)
All	All	1.19	14/9488 (0.1%)	1.30	97/12904 (0.8%)

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 outliers	#Planarity outliers
1	A	0	8
1	B	0	7
1	C	0	7
1	D	0	6
All	All	0	28

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	115	ALA	N-CA	6.62	1.52	1.46
1	B	246	ASN	N-CA	6.60	1.52	1.46
1	D	46	ALA	CA-CB	6.13	1.66	1.53
1	D	193	ILE	CA-CB	5.92	1.61	1.54
1	C	112	TRP	C-O	-5.67	1.17	1.24
1	A	192	GLU	CA-C	-5.60	1.45	1.52
1	C	115	ALA	N-CA	5.58	1.54	1.46
1	B	112	TRP	C-O	-5.55	1.17	1.24
1	B	131	TRP	N-CA	5.49	1.53	1.46
1	D	112	TRP	C-O	-5.47	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	THR	C-O	-5.41	1.20	1.25
1	B	246	ASN	CA-C	5.39	1.58	1.52
1	D	131	TRP	N-CA	5.36	1.53	1.46
1	D	77	PHE	CA-C	-5.33	1.45	1.52

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	244	PHE	N-CA-C	11.41	126.52	112.59
1	C	244	PHE	N-CA-C	11.34	126.42	112.59
1	B	244	PHE	N-CA-C	11.26	126.32	112.59
1	A	244	PHE	N-CA-C	10.82	125.80	112.59
1	A	276	VAL	CB-CA-C	-10.55	94.58	110.82
1	C	25	ASP	N-CA-C	9.29	124.28	111.55
1	B	25	ASP	N-CA-C	9.12	124.65	112.25
1	A	131	TRP	N-CA-C	-8.86	96.51	108.74
1	B	276	VAL	CB-CA-C	-8.80	96.95	110.50
1	C	276	VAL	CB-CA-C	-8.73	97.06	110.50
1	B	274	VAL	CB-CA-C	-8.70	97.65	110.62
1	D	207	THR	CA-C-N	8.57	128.33	119.76
1	D	207	THR	C-N-CA	8.57	128.33	119.76
1	D	276	VAL	CB-CA-C	-8.53	97.37	110.50
1	D	139	ASN	N-CA-C	8.52	128.95	110.80
1	A	274	VAL	CB-CA-C	-8.49	97.43	110.50
1	A	139	ASN	N-CA-C	8.41	128.72	110.80
1	B	139	ASN	N-CA-C	8.06	127.97	110.80
1	C	274	VAL	CB-CA-C	-7.80	98.48	110.50
1	D	131	TRP	N-CA-C	-7.64	98.19	108.74
1	C	139	ASN	N-CA-C	7.57	126.92	110.80
1	B	246	ASN	N-CA-C	7.49	125.86	113.50
1	C	207	THR	CA-C-N	7.46	127.22	119.76
1	C	207	THR	C-N-CA	7.46	127.22	119.76
1	B	211	ARG	NE-CZ-NH1	-7.27	114.23	121.50
1	B	211	ARG	NE-CZ-NH2	7.20	125.68	119.20
1	C	131	TRP	N-CA-C	-7.13	98.89	108.74
1	A	246	ASN	N-CA-C	7.01	125.07	113.50
1	D	274	VAL	CB-CA-C	-7.01	99.71	110.50
1	B	21	GLY	N-CA-C	-6.94	104.52	112.29
1	D	246	ASN	N-CA-C	6.89	124.87	113.50
1	A	244	PHE	CA-C-N	6.69	132.20	122.16
1	A	244	PHE	C-N-CA	6.69	132.20	122.16
1	B	244	PHE	CA-C-N	6.64	132.12	122.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	PHE	C-N-CA	6.64	132.12	122.16
1	C	244	PHE	CA-C-N	6.62	132.10	122.16
1	C	244	PHE	C-N-CA	6.62	132.10	122.16
1	C	246	ASN	N-CA-C	6.61	124.40	113.50
1	C	248	LEU	N-CA-C	-6.55	100.78	110.48
1	C	21	GLY	N-CA-C	-6.50	105.01	112.29
1	B	22	TYR	CA-C-N	6.46	134.07	121.41
1	B	22	TYR	C-N-CA	6.46	134.07	121.41
1	B	131	TRP	N-CA-C	-6.33	99.94	108.86
1	A	207	THR	CA-C-N	6.07	125.83	119.76
1	A	207	THR	C-N-CA	6.07	125.83	119.76
1	C	115	ALA	CA-C-N	-6.00	114.09	120.03
1	C	115	ALA	C-N-CA	-6.00	114.09	120.03
1	D	248	LEU	N-CA-C	-5.98	101.62	110.48
1	B	207	THR	CA-C-N	5.95	126.15	119.90
1	B	207	THR	C-N-CA	5.95	126.15	119.90
1	D	244	PHE	CA-C-N	5.95	132.41	121.70
1	D	244	PHE	C-N-CA	5.95	132.41	121.70
1	B	248	LEU	N-CA-C	-5.86	102.23	110.50
1	C	246	ASN	CA-C-N	5.78	132.11	121.70
1	C	246	ASN	C-N-CA	5.78	132.11	121.70
1	A	132	LEU	N-CA-C	-5.72	99.28	108.55
1	A	272	ALA	CA-C-N	-5.69	113.76	121.27
1	A	272	ALA	C-N-CA	-5.69	113.76	121.27
1	D	168	ARG	NE-CZ-NH1	5.66	127.16	121.50
1	D	130	GLY	CA-C-O	-5.64	116.27	121.63
1	A	184	ASN	N-CA-C	5.64	122.80	110.80
1	D	184	ASN	N-CA-C	5.62	122.76	110.80
1	B	37	ASN	N-CA-C	5.59	117.68	109.24
1	A	183	ARG	CA-C-N	5.51	132.07	121.54
1	A	183	ARG	C-N-CA	5.51	132.07	121.54
1	B	22	TYR	O-C-N	-5.50	115.83	122.65
1	B	138	ALA	CA-C-N	-5.42	111.19	121.54
1	B	138	ALA	C-N-CA	-5.42	111.19	121.54
1	D	168	ARG	CD-NE-CZ	5.37	131.92	124.40
1	B	132	LEU	N-CA-C	-5.33	99.91	108.55
1	A	168	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	D	37	ASN	N-CA-C	5.20	117.09	109.24
1	B	194	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	B	244	PHE	CA-C-O	-5.18	113.83	119.95
1	D	183	ARG	CA-C-N	5.17	131.42	121.54
1	D	183	ARG	C-N-CA	5.17	131.42	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	ARG	CA-C-N	5.17	131.01	121.70
1	C	183	ARG	C-N-CA	5.17	131.01	121.70
1	C	132	LEU	N-CA-C	-5.16	99.92	108.75
1	C	235	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	C	185	ASN	N-CA-C	5.12	117.66	110.23
1	A	246	ASN	CA-C-N	5.12	130.92	121.70
1	A	246	ASN	C-N-CA	5.12	130.92	121.70
1	C	244	PHE	CA-C-O	-5.12	113.91	119.95
1	C	244	PHE	CB-CA-C	-5.10	102.81	111.02
1	A	138	ALA	N-CA-C	5.09	119.24	112.72
1	D	21	GLY	N-CA-C	-5.07	106.61	112.29
1	C	138	ALA	N-CA-C	5.05	119.19	112.72
1	C	114	ILE	N-CA-C	-5.05	101.21	108.53
1	B	183	ARG	CA-C-N	5.04	131.17	121.54
1	B	183	ARG	C-N-CA	5.04	131.17	121.54
1	B	115	ALA	CA-C-N	-5.04	115.04	120.03
1	B	115	ALA	C-N-CA	-5.04	115.04	120.03
1	D	168	ARG	NE-CZ-NH2	-5.02	114.68	119.20
1	C	168	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	D	205	SER	N-CA-C	-5.02	100.11	108.34
1	A	248	LEU	N-CA-C	-5.01	103.07	110.48

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	ARG	Peptide
1	A	244	PHE	Peptide
1	A	25	ASP	Peptide
1	A	263	GLU	Peptide
1	A	264	GLY	Peptide
1	A	276	VAL	Peptide
1	A	4	ASN	Peptide
1	A	40	ASN	Peptide
1	B	183	ARG	Peptide
1	B	22	TYR	Peptide
1	B	244	PHE	Peptide
1	B	25	ASP	Peptide
1	B	264	GLY	Peptide
1	B	4	ASN	Peptide
1	B	40	ASN	Peptide
1	C	183	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	C	244	PHE	Peptide
1	C	25	ASP	Peptide
1	C	263	GLU	Peptide
1	C	264	GLY	Peptide
1	C	4	ASN	Peptide
1	C	40	ASN	Peptide
1	D	183	ARG	Peptide
1	D	244	PHE	Peptide
1	D	25	ASP	Peptide
1	D	276	VAL	Peptide
1	D	4	ASN	Peptide
1	D	40	ASN	Peptide

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	2298	0	2038	85	0
1	B	2298	0	2038	97	0
1	C	2298	0	2038	98	0
1	D	2298	0	2038	91	0
2	A	9	0	0	0	0
2	B	9	0	0	0	0
2	C	8	0	0	0	0
2	D	7	0	0	0	0
3	A	656	0	1271	94	0
3	B	688	0	1333	75	0
3	C	672	0	1302	77	0
3	D	416	0	806	53	0
4	B	11	0	17	1	0
5	A	110	0	0	8	0
5	B	124	0	0	12	0
5	C	112	0	0	11	0
5	D	114	0	0	8	0
All	All	12128	0	12881	549	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 22.

All (549) 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:C:247:GLY:HA2	5:C:2095:HOH:O	1.38	1.22
3:C:1291:LDA:HM13	3:C:1323:LDA:H52	1.23	1.14
3:D:1301:LDA:H102	3:D:1308:LDA:H102	1.28	1.12
1:A:162:ASN:HD22	1:A:164:THR:H	1.02	1.01
1:D:162:ASN:HD22	1:D:164:THR:H	1.07	1.00
3:C:1308:LDA:H101	3:C:1319:LDA:H122	1.45	0.98
1:D:22:TYR:H	3:D:1313:LDA:H101	1.24	0.98
1:C:247:GLY:CA	5:C:2095:HOH:O	2.01	0.97
1:C:4:ASN:ND2	1:C:5:ASP:HA	1.79	0.97
1:B:4:ASN:ND2	1:B:5:ASP:HA	1.79	0.96
1:C:162:ASN:ND2	1:C:164:THR:H	1.63	0.96
3:C:1291:LDA:CM1	3:C:1323:LDA:H52	1.95	0.96
1:B:162:ASN:HD22	1:B:164:THR:H	1.04	0.94
1:C:162:ASN:HD22	1:C:164:THR:H	1.01	0.94
3:A:1318:LDA:HM13	3:A:1319:LDA:HM13	1.49	0.93
3:A:1304:LDA:H123	3:A:1313:LDA:H82	1.51	0.93
1:D:42:PRO:HB3	3:D:1311:LDA:H51	1.51	0.92
1:D:4:ASN:ND2	1:D:5:ASP:HA	1.84	0.92
3:A:1302:LDA:HM23	5:A:2109:HOH:O	1.69	0.91
1:A:162:ASN:ND2	1:A:164:THR:H	1.67	0.91
1:D:263:GLU:CD	5:D:2107:HOH:O	2.00	0.91
1:C:109:MET:SD	1:C:144:THR:HG21	2.11	0.91
1:B:109:MET:SD	1:B:144:THR:HG21	2.12	0.89
1:B:162:ASN:ND2	1:B:164:THR:H	1.69	0.89
3:A:1318:LDA:CM1	3:A:1319:LDA:HM13	2.03	0.88
1:D:109:MET:SD	1:D:144:THR:HG21	2.14	0.87
1:B:23:GLY:HA3	5:B:2013:HOH:O	1.75	0.86
1:A:109:MET:SD	1:A:144:THR:HG21	2.17	0.85
1:D:162:ASN:ND2	1:D:164:THR:H	1.72	0.85
1:D:144:THR:HG23	1:D:146:TYR:CD1	2.12	0.85
1:A:4:ASN:ND2	1:A:5:ASP:HA	1.92	0.84
3:D:1301:LDA:H102	3:D:1308:LDA:C10	2.08	0.84
1:B:144:THR:HG23	1:B:146:TYR:CD1	2.12	0.83
3:A:1307:LDA:H61	3:A:1315:LDA:HM23	1.59	0.83
1:A:217:TRP:CE3	1:A:228:ARG:HG2	2.13	0.83
1:C:217:TRP:CE3	1:C:228:ARG:HG2	2.13	0.83
3:C:1308:LDA:H101	3:C:1319:LDA:C12	2.09	0.83
1:B:206:VAL:HG12	3:B:1322:LDA:H123	1.58	0.83
3:A:413:LDA:H122	3:A:1315:LDA:H112	1.60	0.82
3:B:1294:LDA:H72	3:B:1301:LDA:H72	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:THR:HG23	1:C:146:TYR:CD1	2.15	0.81
1:B:217:TRP:CE3	1:B:228:ARG:HG2	2.16	0.81
3:A:413:LDA:H61	3:A:1315:LDA:H42	1.63	0.81
3:C:1294:LDA:HM12	3:C:1321:LDA:H72	1.62	0.80
3:C:1291:LDA:H32	3:C:1292:LDA:H31	1.61	0.79
3:D:1292:LDA:H32	3:D:1293:LDA:H31	1.63	0.79
3:B:1292:LDA:H32	3:B:1293:LDA:H31	1.63	0.79
3:A:1291:LDA:H32	3:A:1292:LDA:H31	1.64	0.79
3:B:1294:LDA:H92	3:B:1301:LDA:H81	1.64	0.78
3:C:1291:LDA:H61	3:C:1310:LDA:H71	1.65	0.77
1:B:191:GLN:HE22	3:B:1306:LDA:HM21	1.48	0.77
3:D:1301:LDA:C7	3:D:1307:LDA:H81	2.16	0.76
1:A:144:THR:HG23	1:A:146:TYR:CD1	2.20	0.76
5:B:2105:HOH:O	3:C:1281:LDA:HM21	1.85	0.76
3:B:1292:LDA:HM12	3:B:1326:LDA:H81	1.68	0.76
1:A:274:VAL:HG21	3:A:1320:LDA:H82	1.67	0.75
1:C:136:LYS:HZ2	3:C:1307:LDA:H11	1.50	0.75
3:D:1301:LDA:H71	3:D:1307:LDA:H81	1.67	0.75
1:D:217:TRP:CE3	1:D:228:ARG:HG2	2.21	0.75
1:A:224:ASP:OD1	5:A:2082:HOH:O	2.05	0.75
3:B:1329:LDA:C12	3:B:1330:LDA:H82	2.17	0.74
1:C:254:TYR:CD1	3:C:1323:LDA:H111	2.22	0.74
1:D:144:THR:HG23	1:D:146:TYR:HD1	1.50	0.74
3:C:413:LDA:HM22	3:C:1314:LDA:HM21	1.68	0.74
3:C:413:LDA:H61	3:C:1314:LDA:H102	1.70	0.73
3:B:1292:LDA:HM13	3:B:1326:LDA:H61	1.70	0.73
1:C:198:PRO:HA	1:C:207:THR:HB	1.69	0.73
1:D:252:LEU:CD1	1:D:274:VAL:HG13	2.18	0.73
1:D:136:LYS:HZ3	3:D:1306:LDA:H11	1.53	0.73
1:B:57:TYR:HB3	1:D:226:ILE:HD13	1.71	0.73
1:A:162:ASN:HD22	1:A:164:THR:N	1.84	0.73
3:A:1318:LDA:CM1	3:A:1319:LDA:CM1	2.66	0.73
1:A:136:LYS:HZ2	3:A:1308:LDA:H11	1.54	0.72
3:C:1304:LDA:H121	3:C:1311:LDA:H102	1.72	0.72
3:B:1313:LDA:H61	3:B:1319:LDA:H42	1.72	0.72
3:A:1318:LDA:HM13	3:A:1319:LDA:H11	1.73	0.71
3:A:1318:LDA:HM13	3:A:1319:LDA:CM1	2.20	0.71
1:C:162:ASN:HD22	1:C:164:THR:N	1.84	0.71
3:B:1304:LDA:HM11	3:B:1319:LDA:HM21	1.72	0.71
1:A:252:LEU:CD1	1:A:274:VAL:HG13	2.21	0.70
3:B:1328:LDA:H91	3:B:1330:LDA:H41	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:THR:HG21	3:C:1290:LDA:H102	1.74	0.69
1:D:25:ASP:HB2	1:D:29:LEU:HD13	1.74	0.69
1:B:198:PRO:HA	1:B:207:THR:HB	1.73	0.69
1:B:144:THR:HG23	1:B:146:TYR:HD1	1.57	0.69
1:D:22:TYR:N	3:D:1313:LDA:H101	2.05	0.69
1:B:64:THR:O	5:B:2031:HOH:O	2.10	0.69
1:B:201:LEU:HD21	3:B:1322:LDA:H32	1.74	0.69
3:D:1301:LDA:H91	3:D:1308:LDA:H123	1.75	0.69
1:B:162:ASN:HD22	1:B:164:THR:N	1.87	0.69
1:C:254:TYR:CE1	3:C:1323:LDA:H111	2.27	0.68
3:A:1291:LDA:H101	3:A:1319:LDA:H121	1.76	0.68
1:B:183:ARG:HA	1:B:184:ASN:HB2	1.74	0.68
1:C:32:PRO:HB2	3:C:1298:LDA:H21	1.75	0.68
1:C:144:THR:HG23	1:C:146:TYR:HD1	1.56	0.68
1:A:14:TYR:HB2	3:A:1298:LDA:H82	1.76	0.68
1:C:263:GLU:O	1:C:263:GLU:HG2	1.94	0.68
3:A:1319:LDA:H12	3:A:1320:LDA:O1	1.94	0.67
1:D:207:THR:HG21	3:D:1291:LDA:H102	1.76	0.67
1:A:207:THR:HG21	3:A:1290:LDA:H102	1.76	0.67
1:B:160:THR:OG1	5:B:2069:HOH:O	2.13	0.67
1:B:214:LEU:HG	3:B:1301:LDA:HM12	1.77	0.67
1:A:150:ARG:HB2	1:A:175:ARG:O	1.94	0.67
1:D:198:PRO:HA	1:D:207:THR:HB	1.76	0.66
1:C:252:LEU:CD1	1:C:274:VAL:HG13	2.25	0.66
1:C:5:ASP:OD2	5:C:2002:HOH:O	2.12	0.66
1:C:14:TYR:HB2	3:C:1298:LDA:H82	1.77	0.66
1:C:168:ARG:HH11	3:C:1290:LDA:H123	1.61	0.66
1:B:252:LEU:CD1	1:B:274:VAL:HG13	2.25	0.66
1:C:183:ARG:HA	1:C:184:ASN:HB2	1.78	0.66
1:D:76:GLN:O	3:D:1311:LDA:H52	1.95	0.65
3:A:413:LDA:H122	3:A:1315:LDA:H91	1.77	0.65
3:B:1310:LDA:H122	3:B:1311:LDA:H101	1.78	0.65
1:A:32:PRO:HB2	3:A:1298:LDA:H21	1.79	0.65
3:C:1318:LDA:H51	3:C:1327:LDA:H101	1.77	0.65
3:D:1282:LDA:H92	3:D:1305:LDA:H121	1.77	0.65
3:A:1303:LDA:H42	3:A:1313:LDA:H12	1.77	0.65
3:A:1319:LDA:H32	3:A:1320:LDA:HM12	1.79	0.65
3:C:1291:LDA:H12	3:C:1292:LDA:HM23	1.79	0.65
1:D:175:ARG:NH2	5:D:2067:HOH:O	2.22	0.65
1:A:25:ASP:HB2	1:A:29:LEU:HD13	1.78	0.65
3:A:1306:LDA:H42	3:D:1307:LDA:HM11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:PRO:HA	1:A:207:THR:HB	1.79	0.64
3:C:1299:LDA:H71	3:C:1308:LDA:HM22	1.78	0.64
1:B:144:THR:HG22	1:B:146:TYR:H	1.62	0.64
3:B:1329:LDA:H121	3:B:1330:LDA:H82	1.80	0.63
1:D:168:ARG:HH11	3:D:1291:LDA:H123	1.64	0.63
1:B:14:TYR:HB2	3:B:1299:LDA:H82	1.81	0.63
1:D:183:ARG:HA	1:D:184:ASN:HB2	1.79	0.63
1:C:189:SER:O	1:C:216:ARG:HA	1.99	0.63
3:A:1303:LDA:H91	3:A:1313:LDA:H62	1.81	0.63
3:B:1294:LDA:H92	3:B:1301:LDA:C8	2.28	0.63
3:B:1330:LDA:HM22	1:C:242:TYR:OH	1.98	0.63
3:C:1308:LDA:C10	3:C:1319:LDA:H122	2.25	0.62
1:C:40:ASN:C	1:C:40:ASN:HD22	2.07	0.62
3:A:1297:LDA:O1	3:A:1327:LDA:H12	1.99	0.62
1:B:189:SER:O	1:B:216:ARG:HA	1.99	0.62
1:C:25:ASP:HB2	1:C:29:LEU:HD13	1.81	0.62
3:A:413:LDA:H121	3:A:1325:LDA:H121	1.82	0.62
1:D:132:LEU:HD12	1:D:134:MET:HE2	1.82	0.62
1:A:189:SER:O	1:A:216:ARG:HA	2.00	0.62
1:B:169:VAL:HG23	3:B:1306:LDA:H122	1.81	0.62
1:B:206:VAL:HG12	3:B:1322:LDA:C12	2.30	0.62
1:B:274:VAL:HG21	3:B:1329:LDA:H101	1.81	0.62
1:A:183:ARG:HA	1:A:184:ASN:HB2	1.82	0.62
3:D:1292:LDA:HM23	3:D:1293:LDA:HM23	1.82	0.61
1:C:136:LYS:NZ	3:C:1307:LDA:H11	2.15	0.61
1:C:152:GLU:HA	1:C:173:LEU:O	2.00	0.61
1:D:189:SER:O	1:D:216:ARG:HA	2.01	0.61
3:B:1292:LDA:HM23	3:B:1293:LDA:HM23	1.82	0.61
1:D:15:GLU:HB2	1:D:31:GLU:HG3	1.83	0.61
3:A:1304:LDA:C12	3:A:1313:LDA:H82	2.27	0.60
3:A:1318:LDA:HM11	3:A:1319:LDA:CM1	2.31	0.60
1:D:14:TYR:HB2	3:D:1299:LDA:H82	1.82	0.60
1:A:144:THR:HG23	1:A:146:TYR:HD1	1.66	0.60
1:B:44:ARG:NH1	5:B:2019:HOH:O	2.25	0.60
3:A:1297:LDA:HM13	3:A:1327:LDA:HM11	1.83	0.60
1:B:25:ASP:HB2	1:B:29:LEU:HD13	1.82	0.60
1:C:4:ASN:CG	1:C:5:ASP:HA	2.26	0.60
3:D:1295:LDA:CM2	5:D:2039:HOH:O	2.49	0.60
3:A:1300:LDA:HM13	3:A:1309:LDA:H22	1.85	0.59
1:B:252:LEU:HD12	1:B:274:VAL:HG13	1.83	0.59
3:B:1292:LDA:H12	3:B:1293:LDA:HM23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1308:LDA:C10	3:C:1319:LDA:C12	2.80	0.59
1:B:267:ASP:OD1	5:B:2119:HOH:O	2.15	0.59
3:A:1291:LDA:HM23	3:A:1292:LDA:HM23	1.85	0.58
3:B:1292:LDA:HM12	3:B:1326:LDA:C8	2.31	0.58
3:A:1293:LDA:H72	3:A:1300:LDA:H61	1.85	0.58
3:A:1300:LDA:H21	3:A:1324:LDA:H52	1.84	0.58
3:A:1291:LDA:H12	3:A:1292:LDA:HM23	1.84	0.58
1:B:207:THR:HG21	3:B:1291:LDA:H102	1.85	0.58
1:C:274:VAL:HG22	3:C:1281:LDA:H72	1.85	0.58
1:C:150:ARG:HB2	1:C:175:ARG:O	2.04	0.58
3:C:1294:LDA:CM1	3:C:1321:LDA:H72	2.31	0.58
3:D:1292:LDA:H12	3:D:1293:LDA:HM23	1.84	0.58
1:D:144:THR:HG22	1:D:146:TYR:H	1.69	0.58
1:A:168:ARG:HH11	3:A:1290:LDA:H123	1.68	0.58
1:C:144:THR:HG22	1:C:146:TYR:H	1.69	0.58
3:C:1300:LDA:HM13	3:C:1300:LDA:H32	1.85	0.58
1:A:12:ALA:HB2	3:A:1323:LDA:H82	1.86	0.57
1:D:238:LEU:HD23	3:D:1292:LDA:H111	1.86	0.57
1:B:274:VAL:HG22	3:B:1328:LDA:C8	2.34	0.57
1:C:194:ARG:HB3	5:C:2082:HOH:O	2.03	0.57
1:D:162:ASN:HD22	1:D:164:THR:N	1.90	0.57
1:B:4:ASN:CG	1:B:5:ASP:HA	2.30	0.57
3:A:1300:LDA:H31	3:A:1309:LDA:H51	1.86	0.57
1:A:80:ASN:ND2	3:D:1305:LDA:O1	2.38	0.56
1:C:132:LEU:HD12	1:C:134:MET:HE2	1.87	0.56
3:A:1324:LDA:H71	3:A:1326:LDA:H72	1.87	0.56
1:B:32:PRO:HB2	3:B:1299:LDA:H21	1.86	0.56
1:C:201:LEU:HD21	3:C:1320:LDA:HM22	1.87	0.56
1:C:232:ASP:C	1:C:233:PHE:HD1	2.13	0.56
1:D:252:LEU:HD12	1:D:274:VAL:HG13	1.85	0.56
1:A:144:THR:HG22	1:A:146:TYR:H	1.70	0.56
1:A:191:GLN:NE2	3:A:1309:LDA:HM21	2.20	0.56
1:B:168:ARG:HH11	3:B:1291:LDA:H123	1.70	0.56
1:D:191:GLN:HE22	3:D:1307:LDA:HM23	1.70	0.56
1:B:10:ILE:O	1:B:277:ASN:HB2	2.06	0.56
1:C:15:GLU:HB2	1:C:31:GLU:HG3	1.88	0.56
1:D:80:ASN:ND2	3:D:1281:LDA:O1	2.39	0.56
1:C:81:ASP:O	1:C:127:ARG:NH2	2.39	0.56
1:A:6:TRP:O	3:A:1310:LDA:HM12	2.06	0.55
3:A:1300:LDA:H111	3:A:1315:LDA:H82	1.88	0.55
1:B:44:ARG:NH2	5:B:2017:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:TRP:HE1	3:B:1326:LDA:C2	2.18	0.55
3:B:482:LDA:H32	3:B:1315:LDA:HM13	1.87	0.55
3:C:1318:LDA:H31	3:C:1327:LDA:H82	1.87	0.55
1:D:32:PRO:HB2	3:D:1299:LDA:H21	1.87	0.55
3:C:1291:LDA:HM23	3:C:1292:LDA:HM23	1.88	0.55
1:A:8:PHE:CD1	3:A:1310:LDA:HM11	2.42	0.55
1:B:81:ASP:O	1:B:127:ARG:NH2	2.39	0.55
1:D:246:ASN:H	1:D:247:GLY:HA2	1.72	0.55
3:B:1299:LDA:HM21	3:B:1323:LDA:H22	1.88	0.55
1:A:15:GLU:HB2	1:A:31:GLU:HG3	1.88	0.54
1:A:162:ASN:ND2	1:A:164:THR:N	2.49	0.54
1:B:252:LEU:HG	3:B:1328:LDA:H111	1.89	0.54
3:C:1302:LDA:O1	5:C:2110:HOH:O	2.13	0.54
1:B:274:VAL:HG21	3:B:1329:LDA:H81	1.89	0.54
1:C:252:LEU:HD12	1:C:274:VAL:HG13	1.87	0.54
1:B:40:ASN:C	1:B:40:ASN:HD22	2.15	0.54
1:C:236:VAL:HG23	3:C:1323:LDA:H101	1.89	0.54
3:C:1313:LDA:H92	3:C:1315:LDA:H121	1.88	0.54
1:C:254:TYR:HD1	3:C:1323:LDA:H111	1.72	0.54
1:B:15:GLU:HB2	1:B:31:GLU:HG3	1.88	0.54
1:B:238:LEU:HD23	3:B:1292:LDA:H111	1.90	0.54
3:C:1313:LDA:H31	3:C:1315:LDA:H62	1.88	0.54
1:B:114:ILE:HG23	1:B:134:MET:HE3	1.90	0.54
1:D:40:ASN:C	1:D:40:ASN:HD22	2.15	0.54
3:D:1301:LDA:H71	3:D:1307:LDA:C8	2.38	0.53
1:C:277:ASN:HD21	3:C:1328:LDA:H22	1.73	0.53
3:A:1315:LDA:H101	3:A:1324:LDA:H111	1.91	0.53
1:D:150:ARG:HB2	1:D:175:ARG:O	2.08	0.53
1:B:204:HIS:HD2	1:B:240:TYR:OH	1.92	0.53
1:B:217:TRP:CZ3	1:B:228:ARG:HG2	2.43	0.53
1:C:113:LYS:HB2	1:C:135:TYR:CD2	2.43	0.53
1:C:167:LEU:HD23	3:C:1305:LDA:H122	1.90	0.53
1:A:10:ILE:HG23	1:A:36:PHE:HD2	1.73	0.53
1:A:114:ILE:HG23	1:A:134:MET:HE3	1.91	0.53
1:C:67:ASP:C	1:C:67:ASP:OD2	2.51	0.53
1:D:126:LEU:HD22	3:D:1308:LDA:HM21	1.90	0.53
1:A:4:ASN:O	1:A:5:ASP:CG	2.52	0.53
3:A:1298:LDA:HM11	3:A:1322:LDA:O1	2.09	0.53
1:A:246:ASN:H	1:A:247:GLY:HA2	1.73	0.52
1:B:232:ASP:C	1:B:233:PHE:HD1	2.17	0.52
1:D:25:ASP:O	1:D:28:GLY:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ASN:H	1:B:247:GLY:HA2	1.75	0.52
1:D:113:LYS:HB2	1:D:135:TYR:CD2	2.45	0.52
1:D:171:TYR:HB2	3:D:1307:LDA:H91	1.91	0.52
3:D:1301:LDA:H112	3:D:1307:LDA:H122	1.91	0.52
1:B:152:GLU:HA	1:B:173:LEU:O	2.10	0.52
1:A:100:ASP:OD1	1:A:100:ASP:O	2.28	0.52
1:A:280:PHE:C	3:A:1310:LDA:HM13	2.35	0.52
1:B:197:LEU:O	1:B:208:PRO:HD2	2.10	0.52
1:C:162:ASN:ND2	1:C:164:THR:N	2.46	0.52
1:D:44:ARG:NH1	5:D:2015:HOH:O	2.41	0.51
1:A:10:ILE:O	1:A:277:ASN:HB2	2.10	0.51
3:C:1320:LDA:H41	3:C:1326:LDA:H62	1.92	0.51
1:B:258:TRP:HE1	3:B:1326:LDA:H22	1.75	0.51
1:C:100:ASP:OD1	1:C:100:ASP:O	2.29	0.51
3:A:1322:LDA:H11	3:A:1322:LDA:H72	1.91	0.51
1:B:58:SER:O	1:D:228:ARG:HD3	2.10	0.51
1:C:208:PRO:HB2	3:C:1318:LDA:H102	1.93	0.51
1:B:23:GLY:CA	5:B:2013:HOH:O	2.46	0.51
1:C:10:ILE:O	1:C:277:ASN:HB2	2.11	0.51
3:A:1318:LDA:HM11	3:A:1319:LDA:HM13	1.87	0.51
3:C:1313:LDA:HM21	3:C:1315:LDA:H12	1.93	0.51
1:B:185:ASN:HD22	1:B:222:TRP:HE1	1.58	0.51
1:C:204:HIS:HD2	1:C:240:TYR:OH	1.93	0.51
3:A:413:LDA:C12	3:A:1325:LDA:H121	2.40	0.50
3:A:1318:LDA:HM13	3:A:1319:LDA:C1	2.41	0.50
1:D:232:ASP:C	1:D:233:PHE:HD1	2.19	0.50
3:A:413:LDA:H121	3:A:1325:LDA:C12	2.39	0.50
1:B:211:ARG:HG3	1:B:235:ARG:HB3	1.93	0.50
1:A:197:LEU:O	1:A:208:PRO:HD2	2.12	0.50
1:A:238:LEU:HD23	3:A:1291:LDA:H111	1.92	0.50
3:B:1294:LDA:C7	3:B:1301:LDA:H72	2.37	0.50
1:D:4:ASN:HD22	1:D:5:ASP:HA	1.71	0.50
1:D:100:ASP:OD1	1:D:100:ASP:O	2.28	0.50
1:B:35:TYR:OH	1:B:277:ASN:HB3	2.12	0.50
1:B:206:VAL:CG1	3:B:1322:LDA:H123	2.36	0.50
1:C:132:LEU:CD1	1:C:134:MET:HE2	2.42	0.50
1:C:217:TRP:CZ3	1:C:228:ARG:HG2	2.47	0.50
1:A:25:ASP:O	1:A:28:GLY:N	2.41	0.50
1:B:100:ASP:OD1	1:B:100:ASP:O	2.30	0.50
1:A:35:TYR:OH	1:A:277:ASN:HB3	2.12	0.50
1:A:261:HIS:HB2	1:A:264:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:VAL:HG22	3:B:1328:LDA:H81	1.92	0.50
3:B:1313:LDA:H61	3:B:1319:LDA:C4	2.42	0.50
1:D:10:ILE:O	1:D:277:ASN:HB2	2.11	0.50
1:A:67:ASP:OD2	1:A:67:ASP:C	2.55	0.50
1:A:232:ASP:C	1:A:233:PHE:HD1	2.19	0.50
3:A:413:LDA:C12	3:A:1315:LDA:H91	2.41	0.50
1:B:113:LYS:HB2	1:B:135:TYR:CD2	2.47	0.50
3:B:1292:LDA:CM1	3:B:1326:LDA:H81	2.40	0.50
1:C:10:ILE:HG23	1:C:36:PHE:HD2	1.77	0.50
1:B:144:THR:CG2	1:B:146:TYR:CD1	2.89	0.49
3:B:1314:LDA:H51	3:B:1324:LDA:H81	1.93	0.49
1:C:246:ASN:H	1:C:247:GLY:HA2	1.77	0.49
1:D:204:HIS:HD2	1:D:240:TYR:OH	1.95	0.49
3:B:1292:LDA:H42	3:B:1312:LDA:H41	1.94	0.49
1:C:162:ASN:HD22	1:C:162:ASN:C	2.21	0.49
3:C:1318:LDA:HM12	3:C:1327:LDA:H62	1.93	0.49
1:D:69:PRO:HD2	1:D:93:ASN:O	2.12	0.49
1:C:211:ARG:HH22	3:C:1290:LDA:HM12	1.77	0.49
1:D:246:ASN:O	3:D:1309:LDA:HM23	2.12	0.49
3:A:1313:LDA:HM23	5:A:2091:HOH:O	2.11	0.49
1:A:179:MET:CE	3:A:1308:LDA:HM13	2.43	0.49
1:C:114:ILE:HG23	1:C:134:MET:HE3	1.94	0.49
1:D:22:TYR:CE1	1:D:26:MET:HB3	2.47	0.49
1:A:81:ASP:O	1:A:127:ARG:NH2	2.46	0.49
1:C:35:TYR:OH	1:C:277:ASN:HB3	2.12	0.49
1:C:247:GLY:C	5:C:2095:HOH:O	2.44	0.49
1:B:259:GLN:HB2	1:B:267:ASP:HB2	1.95	0.49
1:B:278:TYR:CE1	3:B:1313:LDA:H52	2.49	0.48
1:C:238:LEU:HD23	3:C:1291:LDA:H111	1.96	0.48
1:B:67:ASP:OD2	1:B:67:ASP:C	2.56	0.48
1:D:136:LYS:NZ	5:D:2054:HOH:O	2.34	0.48
1:A:113:LYS:HB2	1:A:135:TYR:CD2	2.48	0.48
1:A:217:TRP:CZ3	1:A:228:ARG:HG2	2.48	0.48
3:B:413:LDA:H122	3:B:413:LDA:H92	1.72	0.48
1:C:154:GLU:HA	1:C:171:TYR:O	2.13	0.48
3:A:1325:LDA:H122	3:A:1325:LDA:H92	1.72	0.48
1:B:25:ASP:O	1:B:28:GLY:N	2.45	0.48
3:A:1300:LDA:HM13	3:A:1309:LDA:C2	2.42	0.48
1:B:150:ARG:HB2	1:B:175:ARG:O	2.13	0.48
3:C:1325:LDA:HM23	5:C:2031:HOH:O	2.13	0.48
3:A:1298:LDA:H12	3:A:1322:LDA:HM23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ILE:HG12	1:B:280:PHE:HE1	1.78	0.48
3:B:1292:LDA:H101	3:B:1328:LDA:H121	1.96	0.48
1:C:25:ASP:O	1:C:28:GLY:N	2.44	0.48
1:C:274:VAL:CG2	3:C:1281:LDA:H72	2.44	0.48
1:D:109:MET:HE1	1:D:146:TYR:CZ	2.49	0.48
1:A:22:TYR:CE1	1:A:26:MET:HB3	2.49	0.48
1:A:121:LYS:NZ	5:A:2045:HOH:O	2.47	0.48
1:A:280:PHE:O	3:A:1310:LDA:HM13	2.14	0.48
3:C:1309:LDA:HM21	3:C:1309:LDA:H21	1.53	0.48
1:A:175:ARG:NH2	5:A:2064:HOH:O	2.42	0.47
3:A:1300:LDA:C3	3:A:1309:LDA:H51	2.43	0.47
1:B:10:ILE:HG23	1:B:36:PHE:HD2	1.78	0.47
1:B:132:LEU:HD12	1:B:134:MET:HE2	1.96	0.47
1:B:214:LEU:CG	3:B:1301:LDA:HM12	2.43	0.47
1:C:229:GLU:HG2	5:C:2085:HOH:O	2.15	0.47
1:D:217:TRP:CZ3	1:D:228:ARG:HG2	2.48	0.47
3:A:413:LDA:H42	3:A:1315:LDA:HM12	1.96	0.47
3:A:1306:LDA:H22	3:D:1307:LDA:HM11	1.95	0.47
3:A:1313:LDA:C12	3:A:1320:LDA:H121	2.45	0.47
1:B:162:ASN:HD22	1:B:162:ASN:C	2.23	0.47
3:B:1329:LDA:C11	3:B:1330:LDA:H82	2.44	0.47
1:D:10:ILE:HG23	1:D:36:PHE:HD2	1.78	0.47
1:A:252:LEU:HD12	1:A:274:VAL:HG13	1.92	0.47
3:A:1322:LDA:HM12	3:A:1322:LDA:H22	1.74	0.47
3:C:1298:LDA:H42	3:C:1298:LDA:HM23	1.96	0.47
1:D:36:PHE:CG	3:D:1312:LDA:H72	2.50	0.47
1:C:246:ASN:N	1:C:246:ASN:HD22	2.13	0.47
1:D:54:PRO:HD2	1:D:64:THR:O	2.14	0.47
1:A:211:ARG:HH22	3:A:1290:LDA:HM12	1.79	0.46
1:B:8:PHE:CD1	3:B:1307:LDA:HM11	2.50	0.46
1:B:162:ASN:ND2	1:B:164:THR:N	2.51	0.46
3:B:1292:LDA:HM13	3:B:1326:LDA:C6	2.43	0.46
3:B:1294:LDA:H72	3:B:1301:LDA:C7	2.38	0.46
1:D:67:ASP:OD2	1:D:67:ASP:C	2.59	0.46
1:D:136:LYS:NZ	3:D:1306:LDA:HM21	2.29	0.46
4:B:1289:TAM:H41	4:B:1289:TAM:H21	1.42	0.46
1:C:22:TYR:CZ	1:C:26:MET:HB3	2.51	0.46
3:A:1318:LDA:HM11	3:A:1319:LDA:HM11	1.97	0.46
1:B:6:TRP:O	3:B:1307:LDA:HM12	2.16	0.46
3:D:1299:LDA:HM22	3:D:1310:LDA:HM12	1.97	0.46
1:A:204:HIS:HD2	1:A:240:TYR:OH	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:PHE:CD1	3:B:1304:LDA:H51	2.51	0.46
1:D:211:ARG:HH22	3:D:1291:LDA:HM12	1.81	0.46
3:A:1313:LDA:H22	3:A:1313:LDA:HM11	1.64	0.46
1:B:223:GLN:OE1	5:B:2094:HOH:O	2.20	0.46
3:B:1329:LDA:H111	3:B:1330:LDA:H82	1.96	0.46
1:D:4:ASN:O	1:D:5:ASP:CG	2.59	0.46
3:B:1310:LDA:H123	3:B:1311:LDA:H81	1.98	0.46
3:B:1300:LDA:H112	3:B:1306:LDA:H112	1.98	0.46
3:C:1291:LDA:HM12	3:C:1323:LDA:C7	2.46	0.46
1:B:280:PHE:C	3:B:1307:LDA:HM13	2.41	0.46
1:C:128:PHE:HE2	3:C:1308:LDA:H111	1.81	0.46
1:D:35:TYR:OH	1:D:277:ASN:HB3	2.16	0.46
1:D:119:ASP:CG	1:D:127:ARG:NH1	2.74	0.46
1:D:132:LEU:CD1	1:D:134:MET:HE2	2.46	0.46
1:A:185:ASN:HD22	1:A:222:TRP:HE1	1.63	0.45
3:A:1310:LDA:HM21	3:A:1310:LDA:H22	1.80	0.45
3:B:1294:LDA:H11	3:B:1301:LDA:HM13	1.98	0.45
3:B:1304:LDA:H42	3:B:1304:LDA:H12	1.80	0.45
1:C:192:GLU:OE1	1:C:194:ARG:HD3	2.17	0.45
3:B:413:LDA:C3	3:B:1315:LDA:O1	2.64	0.45
1:C:267:ASP:OD1	5:C:2104:HOH:O	2.21	0.45
3:C:1294:LDA:H51	3:C:1294:LDA:H22	1.76	0.45
3:D:1295:LDA:H22	3:D:1295:LDA:H51	1.78	0.45
3:D:1301:LDA:H72	3:D:1307:LDA:H81	1.95	0.45
1:B:161:PHE:O	3:B:1327:LDA:H12	2.16	0.45
1:A:180:ASP:OD2	1:A:180:ASP:C	2.59	0.45
1:B:4:ASN:HD22	1:B:5:ASP:HA	1.76	0.45
1:B:22:TYR:CZ	1:B:26:MET:HB3	2.52	0.45
3:C:1303:LDA:CM1	5:C:2080:HOH:O	2.64	0.45
1:C:232:ASP:O	1:C:233:PHE:HD1	1.99	0.45
3:C:1309:LDA:HM23	3:C:1316:LDA:H32	1.98	0.45
1:C:91:PHE:CD1	1:C:91:PHE:C	2.95	0.45
3:C:1290:LDA:H31	3:C:1328:LDA:H123	1.98	0.45
3:C:1312:LDA:H61	3:C:1324:LDA:H82	1.97	0.45
1:D:192:GLU:OE1	1:D:194:ARG:HD3	2.16	0.45
1:B:264:GLY:O	5:B:2118:HOH:O	2.20	0.45
1:D:246:ASN:N	1:D:247:GLY:HA2	2.32	0.45
3:D:1299:LDA:H21	3:D:1299:LDA:HM23	1.78	0.45
1:A:246:ASN:N	1:A:247:GLY:HA2	2.32	0.45
1:B:69:PRO:HD2	1:B:93:ASN:O	2.17	0.45
1:B:175:ARG:NH2	5:B:2074:HOH:O	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PHE:CD1	1:D:134:MET:HE1	2.52	0.44
3:D:1313:LDA:HM12	3:D:1313:LDA:H22	1.43	0.44
1:D:168:ARG:NH1	3:D:1291:LDA:H123	2.30	0.44
1:A:57:TYR:HE2	3:A:1320:LDA:HM22	1.82	0.44
3:B:1310:LDA:C12	3:B:1311:LDA:H101	2.46	0.44
1:C:10:ILE:HG12	1:C:280:PHE:HE1	1.83	0.44
1:B:268:LYS:NZ	5:B:2120:HOH:O	2.50	0.44
1:C:259:GLN:HB2	1:C:267:ASP:HB2	1.99	0.44
1:A:70:GLU:OE2	1:A:92:ARG:NE	2.39	0.44
3:A:413:LDA:H122	3:A:413:LDA:H92	1.70	0.44
1:B:180:ASP:C	1:B:180:ASP:OD2	2.59	0.44
1:C:263:GLU:O	1:C:263:GLU:CG	2.63	0.44
1:A:226:ILE:HG13	5:A:2069:HOH:O	2.18	0.44
1:C:163:GLU:CD	1:C:163:GLU:H	2.26	0.44
3:C:1290:LDA:H21	3:C:1290:LDA:HM21	1.78	0.44
1:C:136:LYS:HD3	3:C:1307:LDA:H11	2.00	0.44
1:A:179:MET:HE1	3:A:1308:LDA:HM13	1.99	0.43
3:A:1316:LDA:O1	5:A:2109:HOH:O	2.20	0.43
1:B:22:TYR:CE1	1:B:26:MET:HB3	2.53	0.43
3:C:1290:LDA:H51	3:C:1290:LDA:H81	1.79	0.43
1:D:81:ASP:O	1:D:127:ARG:NH2	2.51	0.43
1:B:254:TYR:HD1	3:B:1326:LDA:H123	1.83	0.43
3:D:1299:LDA:HM23	3:D:1299:LDA:H42	2.00	0.43
1:A:272:ALA:HB1	3:A:1319:LDA:H102	2.00	0.43
1:B:34:VAL:HG13	3:B:1299:LDA:H31	2.00	0.43
1:B:246:ASN:N	1:B:247:GLY:HA2	2.33	0.43
3:B:1304:LDA:H91	3:B:1319:LDA:H102	2.00	0.43
3:B:1313:LDA:H22	3:B:1313:LDA:HM23	1.76	0.43
1:C:8:PHE:HA	1:C:37:ASN:O	2.18	0.43
3:C:1321:LDA:HM21	3:C:1321:LDA:H22	1.76	0.43
1:D:34:VAL:HG13	3:D:1299:LDA:H31	2.00	0.43
1:D:109:MET:HE1	1:D:146:TYR:CE1	2.53	0.43
1:A:152:GLU:HA	1:A:173:LEU:O	2.18	0.43
3:A:1300:LDA:HM13	3:A:1300:LDA:H22	1.44	0.43
1:C:70:GLU:OE2	1:C:92:ARG:NE	2.49	0.43
3:C:1303:LDA:HM11	5:C:2080:HOH:O	2.18	0.43
1:D:252:LEU:CD1	1:D:274:VAL:CG1	2.94	0.43
1:A:54:PRO:HD2	1:A:64:THR:O	2.19	0.43
1:B:154:GLU:HA	1:B:171:TYR:O	2.18	0.43
1:D:25:ASP:O	1:D:25:ASP:OD2	2.37	0.43
1:A:8:PHE:CE1	3:A:1310:LDA:HM11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLU:OE1	1:A:194:ARG:HD3	2.18	0.43
1:B:178:ASN:HD22	1:B:184:ASN:H	1.65	0.43
1:C:185:ASN:HD22	1:C:222:TRP:HE1	1.67	0.43
1:A:169:VAL:HG23	3:A:1309:LDA:H111	1.99	0.43
1:C:22:TYR:CE1	1:C:26:MET:HB3	2.53	0.43
1:C:136:LYS:CE	3:C:1307:LDA:HM21	2.49	0.43
1:C:252:LEU:HB3	3:C:1291:LDA:H122	2.00	0.43
3:C:1300:LDA:H22	3:C:1300:LDA:HM11	1.31	0.43
1:D:70:GLU:OE2	1:D:92:ARG:NE	2.43	0.43
1:D:160:THR:OG1	5:D:2062:HOH:O	2.20	0.43
3:C:1313:LDA:H31	3:C:1315:LDA:C6	2.49	0.43
1:B:163:GLU:H	1:B:163:GLU:CD	2.27	0.43
1:D:75:TYR:CZ	3:D:1298:LDA:H41	2.54	0.43
3:B:1298:LDA:H72	3:B:1310:LDA:H82	2.01	0.42
1:D:197:LEU:O	1:D:208:PRO:HD2	2.18	0.42
1:A:69:PRO:HD2	1:A:93:ASN:O	2.18	0.42
1:A:216:ARG:HG2	1:A:231:HIS:HB2	2.00	0.42
3:A:1303:LDA:H91	3:A:1313:LDA:H41	2.02	0.42
3:A:1313:LDA:CM2	5:A:2091:HOH:O	2.67	0.42
3:B:1299:LDA:H42	3:B:1299:LDA:HM23	2.01	0.42
1:C:136:LYS:HZ3	3:C:1307:LDA:HM11	1.84	0.42
1:A:78:LEU:O	1:A:84:SER:HA	2.20	0.42
1:C:246:ASN:N	1:C:247:GLY:HA2	2.33	0.42
1:C:272:ALA:HB1	3:C:1281:LDA:H102	2.02	0.42
1:D:62:ARG:NH1	5:D:2023:HOH:O	2.42	0.42
1:D:152:GLU:HA	1:D:173:LEU:O	2.19	0.42
1:B:54:PRO:HD2	1:B:64:THR:O	2.20	0.42
3:C:1300:LDA:HM13	3:C:1300:LDA:C3	2.47	0.42
1:D:31:GLU:HA	1:D:32:PRO:HD2	1.97	0.42
1:B:148:ASP:OD2	1:B:178:ASN:HA	2.19	0.42
1:D:163:GLU:H	1:D:163:GLU:CD	2.28	0.42
3:D:1291:LDA:H51	3:D:1291:LDA:H81	1.81	0.42
1:C:119:ASP:CG	1:C:127:ARG:NH1	2.77	0.42
3:C:1308:LDA:H112	3:C:1308:LDA:H82	1.67	0.42
1:D:174:GLU:OE2	3:D:1295:LDA:H111	2.20	0.42
1:D:252:LEU:HD11	1:D:274:VAL:HG13	1.98	0.42
1:D:8:PHE:HA	1:D:37:ASN:O	2.19	0.42
3:D:1301:LDA:H102	3:D:1308:LDA:C11	2.49	0.42
3:A:1316:LDA:H102	3:D:1298:LDA:H72	2.02	0.42
3:C:413:LDA:H92	3:C:413:LDA:H122	1.69	0.42
3:D:1301:LDA:O1	3:D:1307:LDA:H22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:MET:SD	3:A:1308:LDA:H12	2.60	0.41
1:C:113:LYS:HD2	1:C:135:TYR:HE2	1.85	0.41
1:C:232:ASP:HB2	1:C:260:ASP:HB2	2.02	0.41
3:A:1307:LDA:H82	3:A:1315:LDA:H12	2.02	0.41
3:A:1321:LDA:H62	3:A:1322:LDA:H52	2.02	0.41
3:B:1295:LDA:H22	3:B:1295:LDA:H51	1.74	0.41
3:D:1292:LDA:H12	3:D:1293:LDA:H12	2.02	0.41
1:B:244:PHE:CZ	3:B:1304:LDA:H122	2.56	0.41
3:B:1292:LDA:H12	3:B:1293:LDA:H12	2.00	0.41
1:A:244:PHE:CZ	3:A:1304:LDA:H122	2.55	0.41
3:A:1299:LDA:H52	3:A:1299:LDA:H81	1.49	0.41
3:A:1326:LDA:H41	1:D:123:THR:HG22	2.03	0.41
3:C:1291:LDA:H12	3:C:1292:LDA:H12	2.03	0.41
3:A:1301:LDA:HM11	3:A:1301:LDA:H21	1.82	0.41
1:D:254:TYR:CE1	3:D:1292:LDA:H31	2.56	0.41
1:A:50:TYR:CD2	1:A:50:TYR:C	2.99	0.41
1:B:50:TYR:CD2	1:B:50:TYR:C	2.98	0.41
1:C:156:GLY:HA3	1:C:169:VAL:O	2.20	0.41
1:C:246:ASN:H	1:C:246:ASN:HD22	1.68	0.41
1:D:68:ARG:HA	1:D:93:ASN:O	2.21	0.41
1:A:136:LYS:NZ	3:A:1308:LDA:HM21	2.36	0.41
1:C:75:TYR:CZ	3:C:1297:LDA:H41	2.54	0.41
1:C:76:GLN:HE22	1:C:84:SER:HB3	1.86	0.41
1:C:254:TYR:CE1	3:C:1291:LDA:H31	2.56	0.41
1:D:136:LYS:CE	3:D:1306:LDA:HM21	2.51	0.41
1:D:162:ASN:HD22	1:D:162:ASN:C	2.29	0.41
1:A:76:GLN:HE22	1:A:84:SER:HB3	1.86	0.41
1:A:220:TRP:CZ3	3:A:1294:LDA:H31	2.55	0.41
1:A:244:PHE:HB2	1:A:248:LEU:O	2.21	0.41
3:A:1294:LDA:H22	3:A:1294:LDA:H51	1.81	0.41
3:B:1291:LDA:H51	3:B:1291:LDA:H81	1.84	0.41
1:C:34:VAL:HG13	3:C:1298:LDA:H31	2.02	0.41
1:C:54:PRO:HD2	1:C:64:THR:O	2.21	0.41
1:C:136:LYS:HB2	3:C:1307:LDA:H41	2.03	0.41
1:D:128:PHE:HE2	3:D:1282:LDA:HM23	1.86	0.41
1:A:91:PHE:CD1	1:A:91:PHE:C	2.99	0.41
1:A:163:GLU:CD	1:A:163:GLU:H	2.28	0.41
3:A:1313:LDA:H21	3:A:1313:LDA:HM21	1.59	0.41
3:B:1309:LDA:H102	3:B:1313:LDA:H51	2.02	0.41
3:B:1312:LDA:H31	3:C:1326:LDA:H52	2.03	0.41
3:C:1299:LDA:H52	3:C:1299:LDA:H81	1.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:ASN:N	1:D:246:ASN:HD22	2.19	0.41
1:A:132:LEU:HD12	1:A:134:MET:HE2	2.02	0.40
1:A:254:TYR:CE1	3:A:1291:LDA:H31	2.57	0.40
1:B:220:TRP:CD1	3:B:1320:LDA:H82	2.57	0.40
1:C:220:TRP:CZ3	3:C:1294:LDA:H31	2.56	0.40
1:A:274:VAL:HG21	3:A:1320:LDA:C8	2.46	0.40
3:A:1290:LDA:H21	3:A:1290:LDA:HM21	1.77	0.40
1:C:276:VAL:HG23	3:C:1298:LDA:H112	2.03	0.40
3:D:1291:LDA:H21	3:D:1291:LDA:HM21	1.76	0.40
1:A:162:ASN:HD22	1:A:162:ASN:C	2.29	0.40
3:A:1291:LDA:H12	3:A:1292:LDA:H12	2.03	0.40
3:B:1307:LDA:HM21	3:B:1307:LDA:H22	1.82	0.40
1:D:159:TYR:HB2	3:D:1304:LDA:H101	2.04	0.40
1:A:178:ASN:HD22	1:A:184:ASN:H	1.69	0.40
3:A:1303:LDA:HM11	3:A:1303:LDA:H21	1.95	0.40
3:A:1304:LDA:H42	3:A:1304:LDA:H12	1.85	0.40
1:D:70:GLU:HG2	5:D:2016:HOH:O	2.20	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	275/281 (98%)	259 (94%)	13 (5%)	3 (1%)	11	13
1	B	275/281 (98%)	260 (94%)	14 (5%)	1 (0%)	30	38
1	C	275/281 (98%)	262 (95%)	12 (4%)	1 (0%)	30	38
1	D	275/281 (98%)	259 (94%)	14 (5%)	2 (1%)	18	23
All	All	1100/1124 (98%)	1040 (94%)	53 (5%)	7 (1%)	21	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	MET
1	A	41	GLY
1	A	184	ASN
1	B	184	ASN
1	C	184	ASN
1	D	26	MET
1	D	184	ASN

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	235/239 (98%)	194 (83%)	41 (17%)	2	2
1	B	235/239 (98%)	193 (82%)	42 (18%)	2	2
1	C	235/239 (98%)	190 (81%)	45 (19%)	1	1
1	D	235/239 (98%)	192 (82%)	43 (18%)	2	2
All	All	940/956 (98%)	769 (82%)	171 (18%)	2	2

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	10	ILE
1	A	13	MET
1	A	16	ILE
1	A	24	GLU
1	A	29	LEU
1	A	31	GLU
1	A	34	VAL
1	A	40	ASN
1	A	44	ARG
1	A	50	TYR
1	A	73	VAL
1	A	87	LEU
1	A	101	GLU
1	A	106	THR

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Mol	Chain	Res	Type
1	A	120	VAL
1	A	122	LEU
1	A	143	THR
1	A	144	THR
1	A	157	LEU
1	A	162	ASN
1	A	175	ARG
1	A	193	ILE
1	A	194	ARG
1	A	201	LEU
1	A	205	SER
1	A	206	VAL
1	A	207	THR
1	A	214	LEU
1	A	219	ASN
1	A	228	ARG
1	A	229	GLU
1	A	232	ASP
1	A	245	GLN
1	A	246	ASN
1	A	252	LEU
1	A	263	GLU
1	A	268	LYS
1	A	274	VAL
1	A	276	VAL
1	A	279	SER
1	B	5	ASP
1	B	10	ILE
1	B	13	MET
1	B	16	ILE
1	B	24	GLU
1	B	29	LEU
1	B	34	VAL
1	B	40	ASN
1	B	50	TYR
1	B	73	VAL
1	B	87	LEU
1	B	101	GLU
1	B	106	THR
1	B	113	LYS
1	B	120	VAL
1	B	122	LEU

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Mol	Chain	Res	Type
1	B	143	THR
1	B	144	THR
1	B	150	ARG
1	B	157	LEU
1	B	162	ASN
1	B	163	GLU
1	B	175	ARG
1	B	193	ILE
1	B	201	LEU
1	B	205	SER
1	B	206	VAL
1	B	207	THR
1	B	211	ARG
1	B	214	LEU
1	B	219	ASN
1	B	228	ARG
1	B	229	GLU
1	B	232	ASP
1	B	245	GLN
1	B	246	ASN
1	B	252	LEU
1	B	263	GLU
1	B	268	LYS
1	B	274	VAL
1	B	276	VAL
1	B	279	SER
1	C	5	ASP
1	C	10	ILE
1	C	13	MET
1	C	16	ILE
1	C	24	GLU
1	C	29	LEU
1	C	31	GLU
1	C	34	VAL
1	C	40	ASN
1	C	44	ARG
1	C	50	TYR
1	C	73	VAL
1	C	87	LEU
1	C	101	GLU
1	C	106	THR
1	C	120	VAL

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Mol	Chain	Res	Type
1	C	122	LEU
1	C	142	ASN
1	C	143	THR
1	C	144	THR
1	C	150	ARG
1	C	157	LEU
1	C	162	ASN
1	C	163	GLU
1	C	175	ARG
1	C	193	ILE
1	C	194	ARG
1	C	201	LEU
1	C	205	SER
1	C	206	VAL
1	C	207	THR
1	C	214	LEU
1	C	219	ASN
1	C	228	ARG
1	C	229	GLU
1	C	232	ASP
1	C	245	GLN
1	C	246	ASN
1	C	248	LEU
1	C	252	LEU
1	C	263	GLU
1	C	268	LYS
1	C	274	VAL
1	C	276	VAL
1	C	279	SER
1	D	5	ASP
1	D	10	ILE
1	D	13	MET
1	D	16	ILE
1	D	24	GLU
1	D	29	LEU
1	D	34	VAL
1	D	40	ASN
1	D	44	ARG
1	D	50	TYR
1	D	73	VAL
1	D	87	LEU
1	D	101	GLU

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Mol	Chain	Res	Type
1	D	106	THR
1	D	113	LYS
1	D	120	VAL
1	D	122	LEU
1	D	142	ASN
1	D	143	THR
1	D	144	THR
1	D	150	ARG
1	D	157	LEU
1	D	162	ASN
1	D	163	GLU
1	D	175	ARG
1	D	193	ILE
1	D	194	ARG
1	D	201	LEU
1	D	205	SER
1	D	206	VAL
1	D	207	THR
1	D	214	LEU
1	D	228	ARG
1	D	229	GLU
1	D	232	ASP
1	D	245	GLN
1	D	246	ASN
1	D	252	LEU
1	D	263	GLU
1	D	268	LYS
1	D	274	VAL
1	D	276	VAL
1	D	279	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	40	ASN
1	A	80	ASN
1	A	93	ASN
1	A	108	ASN
1	A	110	GLN
1	A	139	ASN
1	A	162	ASN

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Mol	Chain	Res	Type
1	A	170	ASN
1	A	185	ASN
1	A	204	HIS
1	A	246	ASN
1	B	9	ASN
1	B	40	ASN
1	B	74	HIS
1	B	80	ASN
1	B	93	ASN
1	B	108	ASN
1	B	110	GLN
1	B	139	ASN
1	B	162	ASN
1	B	185	ASN
1	B	204	HIS
1	B	246	ASN
1	C	40	ASN
1	C	74	HIS
1	C	93	ASN
1	C	108	ASN
1	C	110	GLN
1	C	139	ASN
1	C	162	ASN
1	C	185	ASN
1	C	204	HIS
1	C	246	ASN
1	C	277	ASN
1	D	9	ASN
1	D	40	ASN
1	D	74	HIS
1	D	93	ASN
1	D	108	ASN
1	D	110	GLN
1	D	139	ASN
1	D	162	ASN
1	D	170	ASN
1	D	185	ASN
1	D	191	GLN
1	D	204	HIS
1	D	234	ASN
1	D	246	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 186 ligands modelled in this entry, 33 are monoatomic - leaving 153 for Mogul analysis.

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	$\# Z > 2$
3	LDA	D	1302	-	13,15,15	2.19	2 (15%)	14,17,17	0.50	0
3	LDA	C	1324	-	13,15,15	2.07	2 (15%)	14,17,17	0.50	0
3	LDA	D	1298	-	13,15,15	1.97	2 (15%)	14,17,17	0.49	0
3	LDA	D	1306	-	13,15,15	2.28	2 (15%)	14,17,17	1.25	2 (14%)
3	LDA	B	1290	-	13,15,15	2.20	2 (15%)	14,17,17	0.74	1 (7%)
3	LDA	A	1289	-	13,15,15	2.14	2 (15%)	14,17,17	0.62	0
3	LDA	C	1302	-	13,15,15	2.25	2 (15%)	14,17,17	0.48	0
3	LDA	A	1292	-	13,15,15	2.08	2 (15%)	14,17,17	0.59	0
3	LDA	A	1318	-	13,15,15	1.78	2 (15%)	14,17,17	0.67	0
3	LDA	B	1321	-	13,15,15	2.77	5 (38%)	14,17,17	1.26	2 (14%)
3	LDA	C	1318	-	13,15,15	2.05	2 (15%)	14,17,17	0.66	0
3	LDA	C	1306	-	13,15,15	2.46	2 (15%)	14,17,17	0.89	0
3	LDA	B	1323	-	13,15,15	2.33	2 (15%)	14,17,17	0.55	0
3	LDA	C	1321	-	13,15,15	2.11	2 (15%)	14,17,17	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LDA	D	1303	-	13,15,15	2.18	2 (15%)	14,17,17	0.39	0
3	LDA	B	482	-	13,15,15	2.19	2 (15%)	14,17,17	0.70	0
3	LDA	B	1297	-	13,15,15	2.17	2 (15%)	14,17,17	0.50	0
3	LDA	A	1311	-	13,15,15	2.26	2 (15%)	14,17,17	0.58	0
3	LDA	A	1317	-	13,15,15	2.21	2 (15%)	14,17,17	0.54	0
3	LDA	C	1304	-	13,15,15	2.38	2 (15%)	14,17,17	0.46	0
3	LDA	C	1312	-	13,15,15	2.17	2 (15%)	14,17,17	0.44	0
3	LDA	A	1314	-	13,15,15	2.33	2 (15%)	14,17,17	0.49	0
3	LDA	C	1319	-	13,15,15	2.13	2 (15%)	14,17,17	0.81	0
3	LDA	B	1318	-	13,15,15	2.20	2 (15%)	14,17,17	0.46	0
3	LDA	C	1300	-	13,15,15	2.56	2 (15%)	14,17,17	0.53	0
3	LDA	A	1297	-	13,15,15	2.01	2 (15%)	14,17,17	0.47	0
3	LDA	A	1312	-	13,15,15	3.10	2 (15%)	14,17,17	1.94	2 (14%)
3	LDA	A	1304	-	13,15,15	2.86	2 (15%)	14,17,17	1.54	3 (21%)
3	LDA	D	1307	-	13,15,15	2.29	2 (15%)	14,17,17	0.72	0
3	LDA	D	1308	-	13,15,15	2.75	2 (15%)	14,17,17	2.14	2 (14%)
3	LDA	C	1313	-	13,15,15	2.28	2 (15%)	14,17,17	0.58	0
3	LDA	B	1311	-	13,15,15	2.22	2 (15%)	14,17,17	0.72	0
3	LDA	C	1305	-	13,15,15	2.52	2 (15%)	14,17,17	0.51	0
3	LDA	C	1281	-	13,15,15	2.65	2 (15%)	14,17,17	0.53	0
3	LDA	D	1295	-	13,15,15	2.16	2 (15%)	14,17,17	0.69	0
3	LDA	A	1303	-	13,15,15	2.91	2 (15%)	14,17,17	1.12	1 (7%)
3	LDA	C	1323	-	13,15,15	2.24	2 (15%)	14,17,17	0.50	0
3	LDA	B	1330	-	13,15,15	2.33	2 (15%)	14,17,17	0.77	0
3	LDA	A	1316	-	13,15,15	2.21	2 (15%)	14,17,17	0.57	0
3	LDA	B	1327	-	13,15,15	2.35	5 (38%)	14,17,17	0.96	1 (7%)
3	LDA	C	1310	-	13,15,15	2.11	2 (15%)	14,17,17	0.59	0
3	LDA	D	1311	-	13,15,15	2.12	2 (15%)	14,17,17	0.66	0
3	LDA	C	1325	-	13,15,15	1.77	1 (7%)	14,17,17	0.77	1 (7%)
3	LDA	C	1326	-	13,15,15	2.21	2 (15%)	14,17,17	0.70	0
3	LDA	B	1317	-	13,15,15	2.26	2 (15%)	14,17,17	0.48	0
3	LDA	A	1300	-	13,15,15	2.58	2 (15%)	14,17,17	0.55	0
3	LDA	A	1307	-	13,15,15	2.45	2 (15%)	14,17,17	1.41	1 (7%)
3	LDA	A	1308	-	13,15,15	2.16	2 (15%)	14,17,17	1.07	1 (7%)
3	LDA	B	1303	-	13,15,15	2.13	2 (15%)	14,17,17	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LDA	A	1309	-	13,15,15	2.36	2 (15%)	14,17,17	0.71	0
3	LDA	B	1329	-	13,15,15	2.57	2 (15%)	14,17,17	0.59	0
3	LDA	A	1302	-	13,15,15	2.21	2 (15%)	14,17,17	0.47	0
3	LDA	A	1315	-	13,15,15	2.78	2 (15%)	14,17,17	2.04	1 (7%)
3	LDA	D	1293	-	13,15,15	2.23	2 (15%)	14,17,17	0.54	0
3	LDA	B	1299	-	13,15,15	2.27	2 (15%)	14,17,17	0.94	1 (7%)
3	LDA	C	1328	-	13,15,15	2.25	2 (15%)	14,17,17	0.39	0
3	LDA	B	1325	-	13,15,15	2.20	2 (15%)	14,17,17	0.59	0
3	LDA	C	1295	-	13,15,15	2.18	2 (15%)	14,17,17	0.75	0
3	LDA	C	1296	-	13,15,15	2.19	2 (15%)	14,17,17	0.51	0
3	LDA	D	1312	-	13,15,15	2.20	2 (15%)	14,17,17	0.43	0
3	LDA	D	1313	-	13,15,15	2.49	2 (15%)	14,17,17	0.56	0
3	LDA	B	1301	-	13,15,15	2.55	2 (15%)	14,17,17	0.49	0
3	LDA	A	1298	-	13,15,15	2.27	2 (15%)	14,17,17	0.93	1 (7%)
3	LDA	C	1298	-	13,15,15	2.24	2 (15%)	14,17,17	0.93	1 (7%)
3	LDA	B	1324	-	13,15,15	2.19	2 (15%)	14,17,17	0.49	0
3	LDA	A	413	-	13,15,15	2.28	2 (15%)	14,17,17	0.59	0
3	LDA	A	1323	-	13,15,15	2.10	2 (15%)	14,17,17	0.58	0
3	LDA	A	1322	-	13,15,15	2.37	2 (15%)	14,17,17	0.42	0
3	LDA	B	1306	-	13,15,15	2.30	2 (15%)	14,17,17	0.73	0
3	LDA	B	1304	-	13,15,15	2.82	2 (15%)	14,17,17	1.72	3 (21%)
3	LDA	A	1306	-	13,15,15	2.44	2 (15%)	14,17,17	0.53	0
3	LDA	B	1298	-	13,15,15	2.08	2 (15%)	14,17,17	0.57	0
3	LDA	C	1293	-	13,15,15	2.16	2 (15%)	14,17,17	0.59	0
3	LDA	A	1324	-	13,15,15	2.18	2 (15%)	14,17,17	0.59	0
3	LDA	A	1321	-	13,15,15	2.28	2 (15%)	14,17,17	0.53	0
3	LDA	C	1309	-	13,15,15	2.31	2 (15%)	14,17,17	0.62	0
3	LDA	D	1292	-	13,15,15	2.20	2 (15%)	14,17,17	0.65	0
3	LDA	D	1299	-	13,15,15	2.19	2 (15%)	14,17,17	0.87	1 (7%)
3	LDA	D	1296	-	13,15,15	2.15	2 (15%)	14,17,17	0.73	0
3	LDA	C	1307	-	13,15,15	2.21	2 (15%)	14,17,17	1.00	2 (14%)
3	LDA	A	1320	-	13,15,15	2.21	2 (15%)	14,17,17	0.73	0
3	LDA	D	1282	-	13,15,15	1.87	2 (15%)	14,17,17	0.82	1 (7%)
3	LDA	B	1313	-	13,15,15	2.13	2 (15%)	14,17,17	0.50	0
3	LDA	B	1316	-	13,15,15	2.50	2 (15%)	14,17,17	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LDA	A	1296	-	13,15,15	2.10	2 (15%)	14,17,17	0.51	0
3	LDA	A	1326	-	13,15,15	2.32	2 (15%)	14,17,17	0.53	0
3	LDA	B	1296	-	13,15,15	2.17	2 (15%)	14,17,17	0.71	0
3	LDA	D	1297	-	13,15,15	2.12	2 (15%)	14,17,17	0.44	0
3	LDA	B	1300	-	13,15,15	2.40	2 (15%)	14,17,17	0.55	0
3	LDA	B	1308	-	13,15,15	2.14	2 (15%)	14,17,17	0.57	0
3	LDA	C	1311	-	13,15,15	2.23	2 (15%)	14,17,17	0.55	0
3	LDA	A	1305	-	13,15,15	2.22	2 (15%)	14,17,17	0.78	0
3	LDA	B	1307	-	13,15,15	2.03	2 (15%)	14,17,17	0.89	1 (7%)
3	LDA	C	1322	-	13,15,15	2.19	2 (15%)	14,17,17	0.68	0
3	LDA	B	1310	-	13,15,15	2.27	2 (15%)	14,17,17	0.51	0
3	LDA	A	1291	-	13,15,15	2.19	2 (15%)	14,17,17	0.68	0
3	LDA	B	1294	-	13,15,15	2.25	2 (15%)	14,17,17	0.62	0
3	LDA	C	1291	-	13,15,15	2.20	2 (15%)	14,17,17	0.65	0
3	LDA	C	1299	-	13,15,15	2.42	2 (15%)	14,17,17	0.66	0
3	LDA	B	1302	-	13,15,15	2.10	2 (15%)	14,17,17	0.47	0
3	LDA	C	1292	-	13,15,15	2.24	2 (15%)	14,17,17	0.52	0
3	LDA	B	1293	-	13,15,15	2.15	2 (15%)	14,17,17	0.53	0
3	LDA	C	1327	-	13,15,15	2.24	2 (15%)	14,17,17	0.57	0
3	LDA	B	1328	-	13,15,15	2.69	2 (15%)	14,17,17	1.24	2 (14%)
3	LDA	A	1310	-	13,15,15	2.06	2 (15%)	14,17,17	0.98	1 (7%)
3	LDA	C	1290	-	13,15,15	1.97	2 (15%)	14,17,17	0.79	0
3	LDA	A	1299	-	13,15,15	2.29	2 (15%)	14,17,17	0.66	0
3	LDA	B	1292	-	13,15,15	2.14	2 (15%)	14,17,17	0.68	0
3	LDA	C	1308	-	13,15,15	2.22	2 (15%)	14,17,17	0.64	0
3	LDA	A	1301	-	13,15,15	2.22	2 (15%)	14,17,17	0.42	0
3	LDA	D	1290	-	13,15,15	2.27	2 (15%)	14,17,17	0.71	1 (7%)
3	LDA	C	1289	-	13,15,15	2.08	2 (15%)	14,17,17	0.65	0
3	LDA	C	1320	-	13,15,15	2.09	2 (15%)	14,17,17	0.39	0
3	LDA	C	413	-	13,15,15	2.36	2 (15%)	14,17,17	0.56	0
3	LDA	B	1312	-	13,15,15	2.07	2 (15%)	14,17,17	0.61	0
3	LDA	C	1294	-	13,15,15	2.12	2 (15%)	14,17,17	0.73	0
3	LDA	B	1319	-	13,15,15	2.16	2 (15%)	14,17,17	0.69	0
3	LDA	A	1325	-	13,15,15	2.24	2 (15%)	14,17,17	0.57	0
3	LDA	C	1297	-	13,15,15	1.92	2 (15%)	14,17,17	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LDA	D	1304	-	13,15,15	2.62	2 (15%)	14,17,17	1.43	1 (7%)
3	LDA	A	1293	-	13,15,15	2.23	2 (15%)	14,17,17	0.55	0
3	LDA	D	1300	-	13,15,15	2.34	2 (15%)	14,17,17	0.59	0
3	LDA	B	413	-	13,15,15	2.38	2 (15%)	14,17,17	0.61	0
3	LDA	C	1315	-	13,15,15	2.33	2 (15%)	14,17,17	0.56	0
3	LDA	B	1291	-	13,15,15	1.86	2 (15%)	14,17,17	0.73	0
3	LDA	B	1295	-	13,15,15	2.16	2 (15%)	14,17,17	0.85	0
3	LDA	B	1320	-	13,15,15	2.20	2 (15%)	14,17,17	0.52	0
4	TAM	B	1289	-	10,10,10	0.98	1 (10%)	12,12,12	1.19	2 (16%)
3	LDA	D	1305	-	13,15,15	2.69	2 (15%)	14,17,17	1.08	0
3	LDA	C	1317	-	13,15,15	2.23	2 (15%)	14,17,17	0.58	0
3	LDA	D	1281	-	13,15,15	2.63	2 (15%)	14,17,17	1.03	0
3	LDA	A	1028	-	13,15,15	2.14	2 (15%)	14,17,17	0.55	0
3	LDA	D	1294	-	13,15,15	2.19	2 (15%)	14,17,17	0.56	0
3	LDA	A	1290	-	13,15,15	2.03	2 (15%)	14,17,17	0.84	0
3	LDA	B	1309	-	13,15,15	3.05	2 (15%)	14,17,17	1.90	3 (21%)
3	LDA	B	1314	-	13,15,15	2.39	2 (15%)	14,17,17	0.54	0
3	LDA	D	1310	-	13,15,15	2.05	2 (15%)	14,17,17	0.63	0
3	LDA	C	1314	-	13,15,15	2.18	2 (15%)	14,17,17	0.59	0
3	LDA	B	1315	-	13,15,15	2.24	2 (15%)	14,17,17	0.51	0
3	LDA	D	1309	-	13,15,15	2.12	2 (15%)	14,17,17	0.54	0
3	LDA	A	1319	-	13,15,15	2.17	2 (15%)	14,17,17	0.47	0
3	LDA	D	1301	-	13,15,15	2.52	2 (15%)	14,17,17	0.52	0
3	LDA	A	1313	-	13,15,15	2.25	2 (15%)	14,17,17	0.85	0
3	LDA	C	1303	-	13,15,15	2.34	2 (15%)	14,17,17	0.68	0
3	LDA	A	1327	-	13,15,15	2.23	2 (15%)	14,17,17	0.72	0
3	LDA	D	1291	-	13,15,15	1.97	2 (15%)	14,17,17	0.80	0
3	LDA	C	1316	-	13,15,15	2.07	2 (15%)	14,17,17	0.55	0
3	LDA	B	1326	-	13,15,15	2.19	2 (15%)	14,17,17	0.50	0
3	LDA	B	1322	-	13,15,15	2.32	2 (15%)	14,17,17	0.60	0
3	LDA	A	1295	-	13,15,15	2.17	2 (15%)	14,17,17	0.77	0
3	LDA	A	1294	-	13,15,15	2.06	2 (15%)	14,17,17	0.85	0
3	LDA	C	1301	-	13,15,15	2.15	2 (15%)	14,17,17	0.43	0
3	LDA	B	1305	-	13,15,15	2.33	2 (15%)	14,17,17	0.79	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
3	LDA	D	1302	-	-	7/13/13/13	-
3	LDA	C	1324	-	-	3/13/13/13	-
3	LDA	D	1298	-	-	5/13/13/13	-
3	LDA	D	1306	-	-	7/13/13/13	-
3	LDA	B	1290	-	-	11/13/13/13	-
3	LDA	A	1289	-	-	11/13/13/13	-
3	LDA	C	1302	-	-	6/13/13/13	-
3	LDA	A	1292	-	-	7/13/13/13	-
3	LDA	A	1318	-	-	6/13/13/13	-
3	LDA	B	1321	-	-	6/13/13/13	-
3	LDA	C	1318	-	-	11/13/13/13	-
3	LDA	C	1306	-	-	6/13/13/13	-
3	LDA	B	1323	-	-	11/13/13/13	-
3	LDA	C	1321	-	-	11/13/13/13	-
3	LDA	D	1303	-	-	6/13/13/13	-
3	LDA	B	482	-	-	7/13/13/13	-
3	LDA	B	1297	-	-	5/13/13/13	-
3	LDA	A	1311	-	-	7/13/13/13	-
3	LDA	A	1317	-	-	5/13/13/13	-
3	LDA	C	1304	-	-	4/13/13/13	-
3	LDA	C	1312	-	-	7/13/13/13	-
3	LDA	A	1314	-	-	7/13/13/13	-
3	LDA	C	1319	-	-	8/13/13/13	-
3	LDA	B	1318	-	-	9/13/13/13	-
3	LDA	C	1300	-	-	9/13/13/13	-
3	LDA	A	1297	-	-	5/13/13/13	-
3	LDA	A	1312	-	-	12/13/13/13	-
3	LDA	A	1304	-	-	10/13/13/13	-
3	LDA	D	1307	-	-	9/13/13/13	-
3	LDA	D	1308	-	-	9/13/13/13	-
3	LDA	C	1313	-	-	9/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LDA	B	1311	-	-	10/13/13/13	-
3	LDA	C	1305	-	-	8/13/13/13	-
3	LDA	C	1281	-	-	11/13/13/13	-
3	LDA	D	1295	-	-	8/13/13/13	-
3	LDA	A	1303	-	-	8/13/13/13	-
3	LDA	C	1323	-	-	8/13/13/13	-
3	LDA	B	1330	-	-	8/13/13/13	-
3	LDA	A	1316	-	-	6/13/13/13	-
3	LDA	B	1327	-	-	8/13/13/13	-
3	LDA	C	1310	-	-	6/13/13/13	-
3	LDA	D	1311	-	-	11/13/13/13	-
3	LDA	C	1325	-	-	7/13/13/13	-
3	LDA	C	1326	-	-	7/13/13/13	-
3	LDA	B	1317	-	-	10/13/13/13	-
3	LDA	A	1300	-	-	11/13/13/13	-
3	LDA	A	1307	-	-	7/13/13/13	-
3	LDA	A	1308	-	-	7/13/13/13	-
3	LDA	B	1303	-	-	6/13/13/13	-
3	LDA	A	1309	-	-	9/13/13/13	-
3	LDA	B	1329	-	-	10/13/13/13	-
3	LDA	A	1302	-	-	6/13/13/13	-
3	LDA	A	1315	-	-	9/13/13/13	-
3	LDA	D	1293	-	-	7/13/13/13	-
3	LDA	B	1299	-	-	5/13/13/13	-
3	LDA	C	1328	-	-	7/13/13/13	-
3	LDA	B	1325	-	-	6/13/13/13	-
3	LDA	C	1295	-	-	6/13/13/13	-
3	LDA	C	1296	-	-	6/13/13/13	-
3	LDA	D	1312	-	-	1/13/13/13	-
3	LDA	D	1313	-	-	10/13/13/13	-
3	LDA	B	1301	-	-	9/13/13/13	-
3	LDA	A	1298	-	-	5/13/13/13	-
3	LDA	C	1298	-	-	6/13/13/13	-
3	LDA	B	1324	-	-	9/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LDA	A	413	-	-	5/13/13/13	-
3	LDA	A	1323	-	-	9/13/13/13	-
3	LDA	A	1322	-	-	6/13/13/13	-
3	LDA	B	1306	-	-	10/13/13/13	-
3	LDA	B	1304	-	-	10/13/13/13	-
3	LDA	A	1306	-	-	4/13/13/13	-
3	LDA	B	1298	-	-	5/13/13/13	-
3	LDA	C	1293	-	-	8/13/13/13	-
3	LDA	A	1324	-	-	11/13/13/13	-
3	LDA	A	1321	-	-	5/13/13/13	-
3	LDA	C	1309	-	-	9/13/13/13	-
3	LDA	D	1292	-	-	8/13/13/13	-
3	LDA	D	1299	-	-	6/13/13/13	-
3	LDA	D	1296	-	-	6/13/13/13	-
3	LDA	C	1307	-	-	8/13/13/13	-
3	LDA	A	1320	-	-	10/13/13/13	-
3	LDA	D	1282	-	-	7/13/13/13	-
3	LDA	B	1313	-	-	7/13/13/13	-
3	LDA	B	1316	-	-	9/13/13/13	-
3	LDA	A	1296	-	-	6/13/13/13	-
3	LDA	A	1326	-	-	4/13/13/13	-
3	LDA	B	1296	-	-	6/13/13/13	-
3	LDA	D	1297	-	-	6/13/13/13	-
3	LDA	B	1300	-	-	7/13/13/13	-
3	LDA	B	1308	-	-	9/13/13/13	-
3	LDA	C	1311	-	-	8/13/13/13	-
3	LDA	A	1305	-	-	5/13/13/13	-
3	LDA	B	1307	-	-	8/13/13/13	-
3	LDA	C	1322	-	-	7/13/13/13	-
3	LDA	B	1310	-	-	6/13/13/13	-
3	LDA	A	1291	-	-	8/13/13/13	-
3	LDA	B	1294	-	-	8/13/13/13	-
3	LDA	C	1291	-	-	8/13/13/13	-
3	LDA	C	1299	-	-	7/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LDA	B	1302	-	-	7/13/13/13	-
3	LDA	C	1292	-	-	7/13/13/13	-
3	LDA	B	1293	-	-	7/13/13/13	-
3	LDA	C	1327	-	-	8/13/13/13	-
3	LDA	B	1328	-	-	8/13/13/13	-
3	LDA	A	1310	-	-	9/13/13/13	-
3	LDA	C	1290	-	-	9/13/13/13	-
3	LDA	A	1299	-	-	7/13/13/13	-
3	LDA	B	1292	-	-	8/13/13/13	-
3	LDA	C	1308	-	-	10/13/13/13	-
3	LDA	A	1301	-	-	7/13/13/13	-
3	LDA	D	1290	-	-	11/13/13/13	-
3	LDA	C	1289	-	-	11/13/13/13	-
3	LDA	C	1320	-	-	8/13/13/13	-
3	LDA	C	413	-	-	5/13/13/13	-
3	LDA	B	1312	-	-	6/13/13/13	-
3	LDA	C	1294	-	-	9/13/13/13	-
3	LDA	B	1319	-	-	6/13/13/13	-
3	LDA	A	1325	-	-	5/13/13/13	-
3	LDA	C	1297	-	-	5/13/13/13	-
3	LDA	D	1304	-	-	7/13/13/13	-
3	LDA	A	1293	-	-	8/13/13/13	-
3	LDA	D	1300	-	-	7/13/13/13	-
3	LDA	B	413	-	-	5/13/13/13	-
3	LDA	C	1315	-	-	7/13/13/13	-
3	LDA	B	1291	-	-	7/13/13/13	-
3	LDA	B	1295	-	-	7/13/13/13	-
3	LDA	B	1320	-	-	7/13/13/13	-
4	TAM	B	1289	-	-	10/12/12/12	-
3	LDA	D	1305	-	-	8/13/13/13	-
3	LDA	C	1317	-	-	10/13/13/13	-
3	LDA	D	1281	-	-	7/13/13/13	-
3	LDA	A	1028	-	-	9/13/13/13	-
3	LDA	D	1294	-	-	8/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LDA	A	1290	-	-	7/13/13/13	-
3	LDA	B	1309	-	-	9/13/13/13	-
3	LDA	B	1314	-	-	10/13/13/13	-
3	LDA	D	1310	-	-	4/13/13/13	-
3	LDA	C	1314	-	-	5/13/13/13	-
3	LDA	B	1315	-	-	8/13/13/13	-
3	LDA	D	1309	-	-	10/13/13/13	-
3	LDA	A	1319	-	-	3/13/13/13	-
3	LDA	D	1301	-	-	10/13/13/13	-
3	LDA	A	1313	-	-	7/13/13/13	-
3	LDA	C	1303	-	-	5/13/13/13	-
3	LDA	A	1327	-	-	10/13/13/13	-
3	LDA	D	1291	-	-	8/13/13/13	-
3	LDA	C	1316	-	-	7/13/13/13	-
3	LDA	B	1326	-	-	7/13/13/13	-
3	LDA	B	1322	-	-	4/13/13/13	-
3	LDA	A	1295	-	-	6/13/13/13	-
3	LDA	A	1294	-	-	7/13/13/13	-
3	LDA	C	1301	-	-	7/13/13/13	-
3	LDA	B	1305	-	-	5/13/13/13	-

All (310) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1309	LDA	O1-N1	-9.59	1.18	1.42
3	A	1312	LDA	O1-N1	-9.41	1.19	1.42
3	A	1304	LDA	O1-N1	-8.74	1.20	1.42
3	A	1303	LDA	O1-N1	-8.60	1.21	1.42
3	B	1304	LDA	O1-N1	-8.58	1.21	1.42
3	B	1328	LDA	O1-N1	-8.46	1.21	1.42
3	D	1304	LDA	O1-N1	-8.44	1.21	1.42
3	A	1315	LDA	O1-N1	-8.31	1.21	1.42
3	D	1308	LDA	O1-N1	-8.16	1.22	1.42
3	A	1307	LDA	O1-N1	-8.14	1.22	1.42
3	A	1306	LDA	O1-N1	-7.15	1.24	1.42
3	C	1281	LDA	O1-N1	-7.07	1.24	1.42
3	D	1306	LDA	O1-N1	-7.05	1.24	1.42
3	B	1315	LDA	O1-N1	-7.04	1.24	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1305	LDA	C1-N1	-7.02	1.44	1.51
3	C	1307	LDA	O1-N1	-7.02	1.24	1.42
3	C	1304	LDA	O1-N1	-7.01	1.25	1.42
3	D	1281	LDA	O1-N1	-7.01	1.25	1.42
3	A	1300	LDA	O1-N1	-6.97	1.25	1.42
3	A	1308	LDA	O1-N1	-6.97	1.25	1.42
3	C	1302	LDA	O1-N1	-6.95	1.25	1.42
3	C	1300	LDA	O1-N1	-6.95	1.25	1.42
3	B	1329	LDA	O1-N1	-6.94	1.25	1.42
3	A	1326	LDA	O1-N1	-6.93	1.25	1.42
3	D	1301	LDA	O1-N1	-6.91	1.25	1.42
3	B	1301	LDA	O1-N1	-6.89	1.25	1.42
3	C	1305	LDA	O1-N1	-6.89	1.25	1.42
3	D	1290	LDA	O1-N1	-6.89	1.25	1.42
3	D	1293	LDA	O1-N1	-6.88	1.25	1.42
3	A	1298	LDA	O1-N1	-6.85	1.25	1.42
3	B	1316	LDA	O1-N1	-6.84	1.25	1.42
3	C	1327	LDA	O1-N1	-6.82	1.25	1.42
3	C	1298	LDA	O1-N1	-6.82	1.25	1.42
3	D	1312	LDA	O1-N1	-6.82	1.25	1.42
3	C	1296	LDA	O1-N1	-6.81	1.25	1.42
3	B	1314	LDA	O1-N1	-6.81	1.25	1.42
3	C	1292	LDA	O1-N1	-6.81	1.25	1.42
3	B	1321	LDA	O1-N1	-6.80	1.25	1.42
3	B	1297	LDA	O1-N1	-6.79	1.25	1.42
3	B	1299	LDA	O1-N1	-6.79	1.25	1.42
3	B	1290	LDA	O1-N1	-6.79	1.25	1.42
3	A	1311	LDA	O1-N1	-6.78	1.25	1.42
3	B	1294	LDA	O1-N1	-6.77	1.25	1.42
3	B	1323	LDA	O1-N1	-6.76	1.25	1.42
3	D	1294	LDA	O1-N1	-6.75	1.25	1.42
3	C	1311	LDA	O1-N1	-6.75	1.25	1.42
3	D	1292	LDA	O1-N1	-6.75	1.25	1.42
3	C	1309	LDA	O1-N1	-6.74	1.25	1.42
3	A	1322	LDA	O1-N1	-6.74	1.25	1.42
3	B	1322	LDA	O1-N1	-6.73	1.25	1.42
3	C	1328	LDA	O1-N1	-6.73	1.25	1.42
3	B	1317	LDA	O1-N1	-6.71	1.25	1.42
3	C	1306	LDA	O1-N1	-6.71	1.25	1.42
3	B	1293	LDA	O1-N1	-6.71	1.25	1.42
3	D	1303	LDA	O1-N1	-6.70	1.25	1.42
3	C	1313	LDA	O1-N1	-6.69	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1291	LDA	O1-N1	-6.69	1.25	1.42
3	B	1325	LDA	O1-N1	-6.68	1.25	1.42
3	C	1303	LDA	O1-N1	-6.68	1.25	1.42
3	A	1293	LDA	O1-N1	-6.68	1.25	1.42
3	B	1311	LDA	O1-N1	-6.68	1.25	1.42
3	B	1310	LDA	O1-N1	-6.67	1.25	1.42
3	D	1302	LDA	O1-N1	-6.67	1.25	1.42
3	A	1321	LDA	O1-N1	-6.67	1.25	1.42
3	C	1312	LDA	O1-N1	-6.66	1.25	1.42
3	A	1291	LDA	O1-N1	-6.66	1.25	1.42
3	D	1305	LDA	O1-N1	-6.65	1.25	1.42
3	A	1302	LDA	O1-N1	-6.65	1.25	1.42
3	C	1301	LDA	O1-N1	-6.64	1.25	1.42
3	A	1314	LDA	O1-N1	-6.64	1.25	1.42
3	A	1327	LDA	O1-N1	-6.64	1.25	1.42
3	B	1330	LDA	O1-N1	-6.63	1.25	1.42
3	C	1326	LDA	O1-N1	-6.63	1.25	1.42
3	B	1324	LDA	O1-N1	-6.62	1.25	1.42
3	A	1324	LDA	O1-N1	-6.62	1.25	1.42
3	A	1309	LDA	O1-N1	-6.62	1.25	1.42
3	B	1320	LDA	O1-N1	-6.62	1.25	1.42
3	A	1310	LDA	O1-N1	-6.61	1.25	1.42
3	A	1320	LDA	O1-N1	-6.61	1.25	1.42
3	C	1314	LDA	O1-N1	-6.61	1.25	1.42
3	B	1318	LDA	O1-N1	-6.61	1.25	1.42
3	D	1299	LDA	O1-N1	-6.61	1.26	1.42
3	B	1306	LDA	O1-N1	-6.60	1.26	1.42
3	A	1316	LDA	O1-N1	-6.60	1.26	1.42
3	B	1327	LDA	O1-N1	-6.60	1.26	1.42
3	A	1292	LDA	O1-N1	-6.60	1.26	1.42
3	B	1300	LDA	O1-N1	-6.60	1.26	1.42
3	C	1324	LDA	O1-N1	-6.60	1.26	1.42
3	A	1296	LDA	O1-N1	-6.59	1.26	1.42
3	B	1308	LDA	O1-N1	-6.59	1.26	1.42
3	D	1300	LDA	O1-N1	-6.59	1.26	1.42
3	D	1297	LDA	O1-N1	-6.59	1.26	1.42
3	C	1293	LDA	O1-N1	-6.58	1.26	1.42
3	C	1321	LDA	O1-N1	-6.58	1.26	1.42
3	C	1315	LDA	O1-N1	-6.57	1.26	1.42
3	C	1322	LDA	O1-N1	-6.57	1.26	1.42
3	B	1303	LDA	O1-N1	-6.56	1.26	1.42
3	B	1307	LDA	O1-N1	-6.56	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1301	LDA	O1-N1	-6.55	1.26	1.42
3	B	1302	LDA	O1-N1	-6.55	1.26	1.42
3	D	1295	LDA	O1-N1	-6.55	1.26	1.42
3	B	1326	LDA	O1-N1	-6.54	1.26	1.42
3	B	413	LDA	O1-N1	-6.54	1.26	1.42
3	A	1289	LDA	O1-N1	-6.53	1.26	1.42
3	A	1317	LDA	O1-N1	-6.53	1.26	1.42
3	A	1313	LDA	O1-N1	-6.51	1.26	1.42
3	D	1307	LDA	O1-N1	-6.51	1.26	1.42
3	C	1323	LDA	O1-N1	-6.51	1.26	1.42
3	B	482	LDA	O1-N1	-6.51	1.26	1.42
3	C	1310	LDA	O1-N1	-6.49	1.26	1.42
3	D	1311	LDA	O1-N1	-6.48	1.26	1.42
3	C	1320	LDA	O1-N1	-6.46	1.26	1.42
3	C	1317	LDA	O1-N1	-6.46	1.26	1.42
3	A	1028	LDA	O1-N1	-6.46	1.26	1.42
3	C	413	LDA	O1-N1	-6.45	1.26	1.42
3	C	1316	LDA	O1-N1	-6.45	1.26	1.42
3	A	1290	LDA	O1-N1	-6.45	1.26	1.42
3	A	1325	LDA	O1-N1	-6.45	1.26	1.42
3	D	1309	LDA	O1-N1	-6.44	1.26	1.42
3	B	1312	LDA	O1-N1	-6.43	1.26	1.42
3	C	1290	LDA	O1-N1	-6.42	1.26	1.42
3	C	1289	LDA	O1-N1	-6.42	1.26	1.42
3	B	1292	LDA	O1-N1	-6.42	1.26	1.42
3	A	1294	LDA	O1-N1	-6.41	1.26	1.42
3	B	1295	LDA	O1-N1	-6.41	1.26	1.42
3	B	1305	LDA	O1-N1	-6.41	1.26	1.42
3	A	1323	LDA	O1-N1	-6.41	1.26	1.42
3	C	1299	LDA	O1-N1	-6.39	1.26	1.42
3	C	1281	LDA	C1-N1	-6.38	1.44	1.51
3	B	1298	LDA	O1-N1	-6.37	1.26	1.42
3	B	1319	LDA	O1-N1	-6.35	1.26	1.42
3	B	1313	LDA	O1-N1	-6.34	1.26	1.42
3	D	1310	LDA	O1-N1	-6.33	1.26	1.42
3	A	413	LDA	O1-N1	-6.32	1.26	1.42
3	D	1296	LDA	O1-N1	-6.32	1.26	1.42
3	D	1281	LDA	C1-N1	-6.32	1.44	1.51
3	D	1313	LDA	C1-N1	-6.31	1.44	1.51
3	D	1313	LDA	O1-N1	-6.27	1.26	1.42
3	B	1296	LDA	O1-N1	-6.27	1.26	1.42
3	C	1294	LDA	O1-N1	-6.26	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1305	LDA	O1-N1	-6.24	1.26	1.42
3	A	1297	LDA	O1-N1	-6.23	1.26	1.42
3	C	1295	LDA	O1-N1	-6.23	1.26	1.42
3	D	1291	LDA	O1-N1	-6.23	1.26	1.42
3	C	1319	LDA	O1-N1	-6.22	1.26	1.42
3	A	1299	LDA	O1-N1	-6.20	1.26	1.42
3	C	1318	LDA	O1-N1	-6.20	1.27	1.42
3	A	1295	LDA	O1-N1	-6.19	1.27	1.42
3	A	1319	LDA	O1-N1	-6.17	1.27	1.42
3	B	1329	LDA	C1-N1	-6.11	1.45	1.51
3	A	1300	LDA	C1-N1	-6.10	1.45	1.51
3	C	1297	LDA	O1-N1	-6.07	1.27	1.42
3	B	1291	LDA	O1-N1	-6.07	1.27	1.42
3	C	1300	LDA	C1-N1	-6.05	1.45	1.51
3	B	1301	LDA	C1-N1	-6.04	1.45	1.51
3	D	1298	LDA	O1-N1	-6.03	1.27	1.42
3	C	1308	LDA	O1-N1	-6.03	1.27	1.42
3	C	1325	LDA	O1-N1	-6.01	1.27	1.42
3	A	1303	LDA	C1-N1	-5.95	1.45	1.51
3	C	1299	LDA	C1-N1	-5.86	1.45	1.51
3	C	1305	LDA	C1-N1	-5.86	1.45	1.51
3	D	1301	LDA	C1-N1	-5.86	1.45	1.51
3	B	1316	LDA	C1-N1	-5.84	1.45	1.51
3	A	1312	LDA	C1-N1	-5.83	1.45	1.51
3	C	1306	LDA	C1-N1	-5.77	1.45	1.51
3	D	1282	LDA	O1-N1	-5.68	1.28	1.42
3	A	1318	LDA	O1-N1	-5.63	1.28	1.42
3	D	1308	LDA	C1-N1	-5.54	1.45	1.51
3	A	1315	LDA	C1-N1	-5.49	1.45	1.51
3	B	1300	LDA	C1-N1	-5.48	1.45	1.51
3	C	413	LDA	C1-N1	-5.47	1.45	1.51
3	B	413	LDA	C1-N1	-5.46	1.45	1.51
3	A	1304	LDA	C1-N1	-5.42	1.45	1.51
3	B	1304	LDA	C1-N1	-5.40	1.45	1.51
3	A	1299	LDA	C1-N1	-5.38	1.45	1.51
3	B	1305	LDA	C1-N1	-5.36	1.45	1.51
3	A	1309	LDA	C1-N1	-5.29	1.46	1.51
3	B	1309	LDA	C1-N1	-5.20	1.46	1.51
3	A	413	LDA	C1-N1	-5.20	1.46	1.51
3	A	1322	LDA	C1-N1	-5.19	1.46	1.51
3	D	1300	LDA	C1-N1	-5.18	1.46	1.51
3	C	1315	LDA	C1-N1	-5.17	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1314	LDA	C1-N1	-5.15	1.46	1.51
3	C	1303	LDA	C1-N1	-5.12	1.46	1.51
3	C	1308	LDA	C1-N1	-5.12	1.46	1.51
3	B	1330	LDA	C1-N1	-5.07	1.46	1.51
3	D	1307	LDA	C1-N1	-5.02	1.46	1.51
3	A	1306	LDA	C1-N1	-5.00	1.46	1.51
3	A	1314	LDA	C1-N1	-4.98	1.46	1.51
3	B	1306	LDA	C1-N1	-4.95	1.46	1.51
3	A	1305	LDA	C1-N1	-4.94	1.46	1.51
3	B	1322	LDA	C1-N1	-4.91	1.46	1.51
3	B	1323	LDA	C1-N1	-4.91	1.46	1.51
3	C	1304	LDA	C1-N1	-4.81	1.46	1.51
3	A	1313	LDA	C1-N1	-4.81	1.46	1.51
3	A	1325	LDA	C1-N1	-4.79	1.46	1.51
3	C	1309	LDA	C1-N1	-4.77	1.46	1.51
3	C	1295	LDA	C1-N1	-4.75	1.46	1.51
3	A	1295	LDA	C1-N1	-4.73	1.46	1.51
3	B	1328	LDA	C1-N1	-4.72	1.46	1.51
3	C	1323	LDA	C1-N1	-4.72	1.46	1.51
3	A	1321	LDA	C1-N1	-4.70	1.46	1.51
3	C	1313	LDA	C1-N1	-4.70	1.46	1.51
3	A	1319	LDA	C1-N1	-4.66	1.46	1.51
3	B	1310	LDA	C1-N1	-4.60	1.46	1.51
3	B	1296	LDA	C1-N1	-4.60	1.46	1.51
3	A	1326	LDA	C1-N1	-4.56	1.46	1.51
3	B	1321	LDA	C9-C8	4.54	1.74	1.51
3	C	1317	LDA	C1-N1	-4.53	1.46	1.51
3	B	1317	LDA	C1-N1	-4.51	1.46	1.51
3	A	1317	LDA	C1-N1	-4.47	1.46	1.51
3	B	1299	LDA	C1-N1	-4.45	1.46	1.51
3	A	1301	LDA	C1-N1	-4.42	1.46	1.51
3	A	1311	LDA	C1-N1	-4.41	1.46	1.51
3	D	1296	LDA	C1-N1	-4.41	1.46	1.51
3	A	1298	LDA	C1-N1	-4.40	1.46	1.51
3	B	1319	LDA	C1-N1	-4.40	1.46	1.51
3	B	1294	LDA	C1-N1	-4.39	1.47	1.51
3	B	482	LDA	C1-N1	-4.37	1.47	1.51
3	A	1293	LDA	C1-N1	-4.37	1.47	1.51
3	C	1326	LDA	C1-N1	-4.36	1.47	1.51
3	C	1319	LDA	C1-N1	-4.36	1.47	1.51
3	A	1327	LDA	C1-N1	-4.35	1.47	1.51
3	C	1328	LDA	C1-N1	-4.34	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1311	LDA	C1-N1	-4.33	1.47	1.51
3	A	1320	LDA	C1-N1	-4.32	1.47	1.51
3	A	1316	LDA	C1-N1	-4.30	1.47	1.51
3	D	1299	LDA	C1-N1	-4.29	1.47	1.51
3	B	1313	LDA	C1-N1	-4.26	1.47	1.51
3	C	1311	LDA	C1-N1	-4.26	1.47	1.51
3	D	1290	LDA	C1-N1	-4.25	1.47	1.51
3	C	1322	LDA	C1-N1	-4.24	1.47	1.51
3	C	1298	LDA	C1-N1	-4.23	1.47	1.51
3	B	1321	LDA	C1-N1	-4.22	1.47	1.51
3	B	1326	LDA	C1-N1	-4.22	1.47	1.51
3	C	1291	LDA	C1-N1	-4.20	1.47	1.51
3	C	1292	LDA	C1-N1	-4.20	1.47	1.51
3	B	1320	LDA	C1-N1	-4.19	1.47	1.51
3	A	1291	LDA	C1-N1	-4.19	1.47	1.51
3	A	1302	LDA	C1-N1	-4.18	1.47	1.51
3	B	1318	LDA	C1-N1	-4.18	1.47	1.51
3	B	1292	LDA	C1-N1	-4.15	1.47	1.51
3	B	1324	LDA	C1-N1	-4.13	1.47	1.51
3	B	1325	LDA	C1-N1	-4.11	1.47	1.51
3	C	1314	LDA	C1-N1	-4.11	1.47	1.51
3	A	1324	LDA	C1-N1	-4.09	1.47	1.51
3	D	1292	LDA	C1-N1	-4.09	1.47	1.51
3	C	1294	LDA	C1-N1	-4.08	1.47	1.51
3	A	1028	LDA	C1-N1	-4.08	1.47	1.51
3	D	1304	LDA	C1-N1	-4.08	1.47	1.51
3	D	1302	LDA	C1-N1	-4.04	1.47	1.51
3	D	1293	LDA	C1-N1	-4.03	1.47	1.51
3	C	1327	LDA	C1-N1	-4.01	1.47	1.51
3	C	1293	LDA	C1-N1	-4.01	1.47	1.51
3	B	1295	LDA	C1-N1	-3.98	1.47	1.51
3	C	1302	LDA	C1-N1	-3.97	1.47	1.51
3	D	1306	LDA	C1-N1	-3.97	1.47	1.51
3	B	1290	LDA	C1-N1	-3.96	1.47	1.51
3	C	1312	LDA	C1-N1	-3.92	1.47	1.51
3	D	1309	LDA	C1-N1	-3.91	1.47	1.51
3	D	1294	LDA	C1-N1	-3.91	1.47	1.51
3	C	1318	LDA	C1-N1	-3.90	1.47	1.51
3	D	1311	LDA	C1-N1	-3.90	1.47	1.51
3	A	1323	LDA	C1-N1	-3.89	1.47	1.51
3	B	1308	LDA	C1-N1	-3.89	1.47	1.51
3	A	1289	LDA	C1-N1	-3.88	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1303	LDA	C1-N1	-3.88	1.47	1.51
3	C	1296	LDA	C1-N1	-3.82	1.47	1.51
3	B	1298	LDA	C1-N1	-3.81	1.47	1.51
3	D	1295	LDA	C1-N1	-3.80	1.47	1.51
3	C	1301	LDA	C1-N1	-3.75	1.47	1.51
3	B	1293	LDA	C1-N1	-3.75	1.47	1.51
3	B	1303	LDA	C1-N1	-3.75	1.47	1.51
3	B	1297	LDA	C1-N1	-3.75	1.47	1.51
3	C	1310	LDA	C1-N1	-3.74	1.47	1.51
3	D	1297	LDA	C1-N1	-3.73	1.47	1.51
3	C	1289	LDA	C1-N1	-3.71	1.47	1.51
3	B	1315	LDA	C1-N1	-3.68	1.47	1.51
3	D	1312	LDA	C1-N1	-3.63	1.47	1.51
3	D	1310	LDA	C1-N1	-3.62	1.47	1.51
3	C	1316	LDA	C1-N1	-3.60	1.47	1.51
3	B	1302	LDA	C1-N1	-3.60	1.47	1.51
3	D	1298	LDA	C1-N1	-3.58	1.47	1.51
3	C	1321	LDA	C1-N1	-3.58	1.47	1.51
3	B	1312	LDA	C1-N1	-3.53	1.47	1.51
3	A	1296	LDA	C1-N1	-3.52	1.47	1.51
3	A	1297	LDA	C1-N1	-3.50	1.47	1.51
3	C	1320	LDA	C1-N1	-3.48	1.47	1.51
3	A	1292	LDA	C1-N1	-3.48	1.47	1.51
3	C	1307	LDA	C1-N1	-3.47	1.47	1.51
3	D	1282	LDA	C1-N1	-3.37	1.48	1.51
3	B	1327	LDA	C1-N1	-3.33	1.48	1.51
3	A	1308	LDA	C1-N1	-3.28	1.48	1.51
3	A	1294	LDA	C1-N1	-3.27	1.48	1.51
3	A	1307	LDA	C1-N1	-3.26	1.48	1.51
3	A	1290	LDA	C1-N1	-3.24	1.48	1.51
3	D	1291	LDA	C1-N1	-3.24	1.48	1.51
3	A	1310	LDA	C1-N1	-3.22	1.48	1.51
3	C	1297	LDA	C1-N1	-3.14	1.48	1.51
3	B	1307	LDA	C1-N1	-2.95	1.48	1.51
3	C	1324	LDA	C1-N1	-2.95	1.48	1.51
3	C	1290	LDA	C1-N1	-2.91	1.48	1.51
3	A	1318	LDA	C1-N1	-2.82	1.48	1.51
3	B	1291	LDA	C1-N1	-2.65	1.48	1.51
3	B	1327	LDA	C6-C5	2.52	1.64	1.51
3	B	1321	LDA	C6-C5	2.23	1.62	1.51
3	B	1327	LDA	C8-C7	2.07	1.62	1.51
3	B	1321	LDA	C10-C9	2.06	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1327	LDA	C9-C8	2.04	1.61	1.51
4	B	1289	TAM	C1-C4	2.01	1.55	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1308	LDA	CM2-N1-C1	7.24	125.45	110.23
3	A	1315	LDA	CM2-N1-C1	7.23	125.43	110.23
3	D	1304	LDA	CM1-N1-C1	5.09	120.93	110.23
3	A	1307	LDA	CM1-N1-C1	4.97	120.67	110.23
3	A	1312	LDA	CM1-N1-C1	4.74	120.19	110.23
3	B	1309	LDA	CM1-N1-C1	4.46	119.60	110.23
3	A	1312	LDA	O1-N1-C1	-4.41	98.44	109.27
3	B	1309	LDA	O1-N1-C1	-4.25	98.86	109.27
3	B	1304	LDA	O1-N1-C1	-3.80	99.95	109.27
3	B	1304	LDA	CM2-N1-C1	3.54	117.68	110.23
3	D	1306	LDA	C5-C4-C3	3.52	132.14	114.37
3	A	1304	LDA	CM2-N1-C1	3.44	117.47	110.23
3	B	1321	LDA	C10-C9-C8	-2.96	99.39	114.37
3	A	1304	LDA	O1-N1-C1	-2.87	102.23	109.27
3	A	1310	LDA	CM2-N1-C1	2.82	116.15	110.23
3	D	1306	LDA	CM2-N1-C1	2.69	115.88	110.23
3	B	1328	LDA	CM2-N1-C1	2.67	115.84	110.23
3	B	1304	LDA	CM1-N1-C1	2.61	115.72	110.23
3	B	1307	LDA	CM2-N1-C1	2.60	115.70	110.23
3	B	1299	LDA	CM2-N1-C1	2.52	115.52	110.23
3	A	1308	LDA	CM2-N1-C1	2.51	115.52	110.23
4	B	1289	TAM	C4-C1-C	-2.50	113.02	115.97
3	A	1303	LDA	CM2-N1-C1	2.46	115.40	110.23
3	C	1298	LDA	CM2-N1-C1	2.42	115.32	110.23
3	A	1298	LDA	CM2-N1-C1	2.39	115.26	110.23
3	B	1321	LDA	C9-C8-C7	-2.38	102.31	114.37
3	A	1304	LDA	CM1-N1-C1	2.33	115.12	110.23
3	D	1308	LDA	O1-N1-C1	-2.31	103.60	109.27
4	B	1289	TAM	C5-C2-C	-2.31	113.24	115.97
3	B	1328	LDA	C7-C6-C5	-2.29	102.82	114.37
3	B	1290	LDA	CM1-N1-C1	2.28	115.02	110.23
3	D	1282	LDA	O1-N1-C1	2.26	114.81	109.27
3	C	1307	LDA	CM2-N1-C1	2.25	114.97	110.23
3	D	1290	LDA	CM1-N1-C1	2.24	114.93	110.23
3	D	1299	LDA	CM2-N1-C1	2.15	114.75	110.23
3	B	1327	LDA	C9-C8-C7	-2.12	103.63	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1309	LDA	CM2-N1-C1	2.12	114.68	110.23
3	C	1307	LDA	C5-C4-C3	2.06	124.79	114.37
3	C	1325	LDA	O1-N1-C1	2.02	114.22	109.27

There are no chirality outliers.

All (1139) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1028	LDA	C2-C1-N1-CM1
3	A	1028	LDA	C2-C1-N1-CM2
3	A	1289	LDA	C2-C1-N1-O1
3	A	1289	LDA	C2-C1-N1-CM1
3	A	1289	LDA	C2-C1-N1-CM2
3	A	1289	LDA	N1-C1-C2-C3
3	A	1290	LDA	C2-C1-N1-O1
3	A	1290	LDA	C2-C1-N1-CM1
3	A	1290	LDA	C2-C1-N1-CM2
3	A	1293	LDA	C2-C1-N1-CM1
3	A	1293	LDA	C2-C1-N1-CM2
3	A	1294	LDA	C2-C1-N1-CM1
3	A	1294	LDA	C2-C1-N1-CM2
3	A	1298	LDA	C2-C1-N1-CM2
3	A	1298	LDA	N1-C1-C2-C3
3	A	1300	LDA	C2-C1-N1-O1
3	A	1300	LDA	C2-C1-N1-CM1
3	A	1300	LDA	C2-C1-N1-CM2
3	A	1304	LDA	C2-C1-N1-O1
3	A	1304	LDA	C2-C1-N1-CM1
3	A	1304	LDA	C2-C1-N1-CM2
3	A	1308	LDA	C2-C1-N1-CM1
3	A	1310	LDA	C2-C1-N1-O1
3	A	1310	LDA	C2-C1-N1-CM2
3	A	1312	LDA	N1-C1-C2-C3
3	A	1314	LDA	N1-C1-C2-C3
3	A	1318	LDA	N1-C1-C2-C3
3	A	1320	LDA	C2-C1-N1-O1
3	A	1320	LDA	C2-C1-N1-CM2
3	A	1323	LDA	C2-C1-N1-CM1
3	A	1323	LDA	C2-C1-N1-CM2
3	A	1324	LDA	N1-C1-C2-C3
3	A	1327	LDA	C2-C1-N1-O1
3	A	1327	LDA	C2-C1-N1-CM1

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Mol	Chain	Res	Type	Atoms
3	A	1327	LDA	C2-C1-N1-CM2
3	B	1290	LDA	C2-C1-N1-O1
3	B	1290	LDA	C2-C1-N1-CM1
3	B	1290	LDA	C2-C1-N1-CM2
3	B	1290	LDA	N1-C1-C2-C3
3	B	1291	LDA	C2-C1-N1-O1
3	B	1291	LDA	C2-C1-N1-CM1
3	B	1291	LDA	C2-C1-N1-CM2
3	B	1294	LDA	C2-C1-N1-CM1
3	B	1294	LDA	C2-C1-N1-CM2
3	B	1295	LDA	C2-C1-N1-CM1
3	B	1295	LDA	C2-C1-N1-CM2
3	B	1299	LDA	C2-C1-N1-CM2
3	B	1299	LDA	N1-C1-C2-C3
3	B	1301	LDA	C2-C1-N1-O1
3	B	1301	LDA	C2-C1-N1-CM2
3	B	1304	LDA	C2-C1-N1-O1
3	B	1304	LDA	C2-C1-N1-CM1
3	B	1304	LDA	C2-C1-N1-CM2
3	B	1307	LDA	C2-C1-N1-O1
3	B	1307	LDA	C2-C1-N1-CM2
3	B	1309	LDA	C2-C1-N1-CM2
3	B	1309	LDA	N1-C1-C2-C3
3	B	1311	LDA	C2-C1-N1-O1
3	B	1311	LDA	C2-C1-N1-CM1
3	B	1311	LDA	C2-C1-N1-CM2
3	B	1312	LDA	C2-C1-N1-CM1
3	B	1312	LDA	C2-C1-N1-CM2
3	B	1313	LDA	N1-C1-C2-C3
3	B	1314	LDA	C2-C1-N1-CM1
3	B	1314	LDA	C2-C1-N1-CM2
3	B	1315	LDA	C2-C1-N1-CM1
3	B	1315	LDA	C2-C1-N1-CM2
3	B	1316	LDA	C2-C1-N1-CM2
3	B	1317	LDA	C2-C1-N1-CM2
3	B	1318	LDA	C2-C1-N1-CM1
3	B	1320	LDA	C2-C1-N1-CM2
3	B	1321	LDA	C2-C1-N1-CM2
3	B	1323	LDA	C2-C1-N1-CM1
3	B	1324	LDA	C2-C1-N1-O1
3	B	1324	LDA	C2-C1-N1-CM2
3	B	1325	LDA	N1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	1326	LDA	C2-C1-N1-CM2
3	B	1326	LDA	N1-C1-C2-C3
3	B	1327	LDA	C2-C1-N1-O1
3	B	1327	LDA	C2-C1-N1-CM1
3	B	1327	LDA	C2-C1-N1-CM2
3	B	1329	LDA	C2-C1-N1-O1
3	B	1329	LDA	C2-C1-N1-CM1
3	B	1329	LDA	C2-C1-N1-CM2
3	C	1281	LDA	C2-C1-N1-CM2
3	C	1289	LDA	C2-C1-N1-O1
3	C	1289	LDA	C2-C1-N1-CM1
3	C	1289	LDA	C2-C1-N1-CM2
3	C	1289	LDA	N1-C1-C2-C3
3	C	1290	LDA	C2-C1-N1-O1
3	C	1290	LDA	C2-C1-N1-CM1
3	C	1290	LDA	C2-C1-N1-CM2
3	C	1293	LDA	C2-C1-N1-CM1
3	C	1293	LDA	C2-C1-N1-CM2
3	C	1294	LDA	C2-C1-N1-CM1
3	C	1294	LDA	C2-C1-N1-CM2
3	C	1298	LDA	C2-C1-N1-CM2
3	C	1298	LDA	N1-C1-C2-C3
3	C	1300	LDA	C2-C1-N1-O1
3	C	1300	LDA	C2-C1-N1-CM1
3	C	1300	LDA	C2-C1-N1-CM2
3	C	1300	LDA	N1-C1-C2-C3
3	C	1305	LDA	C2-C1-N1-CM1
3	C	1305	LDA	C2-C1-N1-CM2
3	C	1307	LDA	C2-C1-N1-CM1
3	C	1308	LDA	C2-C1-N1-CM1
3	C	1308	LDA	C2-C1-N1-CM2
3	C	1309	LDA	C2-C1-N1-O1
3	C	1309	LDA	C2-C1-N1-CM1
3	C	1309	LDA	C2-C1-N1-CM2
3	C	1309	LDA	N1-C1-C2-C3
3	C	1312	LDA	C2-C1-N1-O1
3	C	1312	LDA	C2-C1-N1-CM1
3	C	1312	LDA	C2-C1-N1-CM2
3	C	1313	LDA	C2-C1-N1-CM1
3	C	1313	LDA	C2-C1-N1-CM2
3	C	1317	LDA	C2-C1-N1-CM1
3	C	1317	LDA	C2-C1-N1-CM2

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Mol	Chain	Res	Type	Atoms
3	C	1318	LDA	C2-C1-N1-CM1
3	C	1318	LDA	C2-C1-N1-CM2
3	C	1318	LDA	N1-C1-C2-C3
3	C	1319	LDA	C2-C1-N1-CM1
3	C	1319	LDA	C2-C1-N1-CM2
3	C	1320	LDA	C2-C1-N1-CM1
3	C	1320	LDA	C2-C1-N1-CM2
3	C	1321	LDA	C2-C1-N1-O1
3	C	1321	LDA	C2-C1-N1-CM2
3	C	1321	LDA	N1-C1-C2-C3
3	C	1323	LDA	C2-C1-N1-CM2
3	C	1323	LDA	N1-C1-C2-C3
3	C	1326	LDA	C2-C1-N1-CM2
3	C	1327	LDA	C2-C1-N1-O1
3	C	1327	LDA	C2-C1-N1-CM2
3	C	1328	LDA	N1-C1-C2-C3
3	D	1290	LDA	C2-C1-N1-O1
3	D	1290	LDA	C2-C1-N1-CM1
3	D	1290	LDA	C2-C1-N1-CM2
3	D	1290	LDA	N1-C1-C2-C3
3	D	1291	LDA	C2-C1-N1-O1
3	D	1291	LDA	C2-C1-N1-CM1
3	D	1291	LDA	C2-C1-N1-CM2
3	D	1294	LDA	C2-C1-N1-CM1
3	D	1294	LDA	C2-C1-N1-CM2
3	D	1295	LDA	C2-C1-N1-O1
3	D	1295	LDA	C2-C1-N1-CM1
3	D	1295	LDA	C2-C1-N1-CM2
3	D	1299	LDA	C2-C1-N1-CM2
3	D	1299	LDA	N1-C1-C2-C3
3	D	1301	LDA	C2-C1-N1-O1
3	D	1301	LDA	C2-C1-N1-CM1
3	D	1301	LDA	C2-C1-N1-CM2
3	D	1301	LDA	N1-C1-C2-C3
3	D	1306	LDA	C2-C1-N1-CM1
3	D	1308	LDA	C2-C1-N1-O1
3	D	1309	LDA	C2-C1-N1-CM2
3	D	1313	LDA	C2-C1-N1-O1
3	D	1313	LDA	C2-C1-N1-CM1
3	D	1313	LDA	C2-C1-N1-CM2
4	B	1289	TAM	C2-C-C1-C4
4	B	1289	TAM	C3-C-C1-C4

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Mol	Chain	Res	Type	Atoms
4	B	1289	TAM	N-C-C1-C4
4	B	1289	TAM	C1-C-C2-C5
4	B	1289	TAM	C3-C-C2-C5
4	B	1289	TAM	N-C-C2-C5
4	B	1289	TAM	C1-C-C3-C6
4	B	1289	TAM	C2-C-C3-C6
4	B	1289	TAM	N-C-C3-C6
3	A	1294	LDA	C7-C8-C9-C10
3	D	1295	LDA	C7-C8-C9-C10
3	C	1294	LDA	C7-C8-C9-C10
3	A	1300	LDA	C1-C2-C3-C4
3	D	1282	LDA	C4-C5-C6-C7
3	C	1308	LDA	C5-C6-C7-C8
3	B	1304	LDA	C3-C4-C5-C6
3	D	1303	LDA	C4-C5-C6-C7
3	A	1302	LDA	C4-C5-C6-C7
3	A	1304	LDA	C3-C4-C5-C6
3	A	1312	LDA	C6-C7-C8-C9
3	C	1302	LDA	C4-C5-C6-C7
3	C	1308	LDA	C11-C10-C9-C8
3	B	1295	LDA	C7-C8-C9-C10
3	C	1325	LDA	C2-C3-C4-C5
3	A	1317	LDA	C2-C3-C4-C5
3	A	1312	LDA	C1-C2-C3-C4
3	B	1303	LDA	C4-C5-C6-C7
3	C	1281	LDA	C5-C6-C7-C8
3	D	1300	LDA	C5-C6-C7-C8
3	C	1290	LDA	C5-C6-C7-C8
3	C	1299	LDA	C5-C6-C7-C8
3	A	1313	LDA	C1-C2-C3-C4
3	A	1290	LDA	C5-C6-C7-C8
3	B	1300	LDA	C5-C6-C7-C8
3	C	1320	LDA	C9-C10-C11-C12
3	A	1299	LDA	C5-C6-C7-C8
3	B	1291	LDA	C5-C6-C7-C8
3	D	1291	LDA	C5-C6-C7-C8
3	B	1309	LDA	C6-C7-C8-C9
3	A	1301	LDA	C6-C7-C8-C9
3	A	1315	LDA	C11-C10-C9-C8
3	B	1317	LDA	C4-C5-C6-C7
3	C	1316	LDA	C11-C10-C9-C8
3	D	1308	LDA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
3	A	1297	LDA	C6-C7-C8-C9
3	A	1310	LDA	C6-C7-C8-C9
3	A	1312	LDA	C3-C4-C5-C6
3	B	1302	LDA	C6-C7-C8-C9
3	B	1306	LDA	C6-C7-C8-C9
3	B	1326	LDA	C2-C3-C4-C5
3	C	413	LDA	C11-C10-C9-C8
3	C	1311	LDA	C11-C10-C9-C8
3	C	1322	LDA	C2-C3-C4-C5
3	C	1328	LDA	C7-C8-C9-C10
3	D	1311	LDA	C3-C4-C5-C6
3	A	1303	LDA	C5-C6-C7-C8
3	A	1303	LDA	C7-C8-C9-C10
3	A	1316	LDA	C6-C7-C8-C9
3	D	1302	LDA	C6-C7-C8-C9
3	A	1291	LDA	C11-C10-C9-C8
3	A	1312	LDA	C4-C5-C6-C7
3	A	1316	LDA	C2-C3-C4-C5
3	A	1319	LDA	C2-C3-C4-C5
3	A	1324	LDA	C11-C10-C9-C8
3	A	1325	LDA	C11-C10-C9-C8
3	B	1309	LDA	C3-C4-C5-C6
3	B	1310	LDA	C7-C8-C9-C10
3	B	1328	LDA	C3-C4-C5-C6
3	B	1330	LDA	C4-C5-C6-C7
3	C	1301	LDA	C6-C7-C8-C9
3	C	1310	LDA	C7-C8-C9-C10
3	D	1293	LDA	C5-C6-C7-C8
3	D	1298	LDA	C5-C6-C7-C8
3	D	1307	LDA	C6-C7-C8-C9
3	A	413	LDA	C11-C10-C9-C8
3	A	1309	LDA	C6-C7-C8-C9
3	B	413	LDA	C11-C10-C9-C8
3	B	1293	LDA	C5-C6-C7-C8
3	B	1316	LDA	C6-C7-C8-C9
3	A	1324	LDA	C6-C7-C8-C9
3	B	1296	LDA	C6-C7-C8-C9
3	D	1292	LDA	C11-C10-C9-C8
3	B	1292	LDA	C11-C10-C9-C8
3	B	1299	LDA	C2-C3-C4-C5
3	B	1328	LDA	C5-C6-C7-C8
3	A	1308	LDA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	A	1327	LDA	C7-C8-C9-C10
3	B	1328	LDA	C7-C8-C9-C10
3	C	1318	LDA	C4-C5-C6-C7
3	C	1318	LDA	C6-C7-C8-C9
3	A	1028	LDA	C4-C5-C6-C7
3	A	1292	LDA	C5-C6-C7-C8
3	A	1303	LDA	C3-C4-C5-C6
3	A	1314	LDA	C11-C10-C9-C8
3	A	1323	LDA	C2-C3-C4-C5
3	A	1323	LDA	C7-C8-C9-C10
3	B	1294	LDA	C3-C4-C5-C6
3	B	1316	LDA	C2-C3-C4-C5
3	B	1324	LDA	C6-C7-C8-C9
3	C	1292	LDA	C5-C6-C7-C8
3	C	1297	LDA	C6-C7-C8-C9
3	C	1307	LDA	C3-C4-C5-C6
3	C	1320	LDA	C11-C10-C9-C8
3	A	1322	LDA	C7-C8-C9-C10
3	C	1298	LDA	C2-C3-C4-C5
3	C	1311	LDA	C7-C8-C9-C10
3	C	1313	LDA	C11-C10-C9-C8
3	D	1282	LDA	C11-C10-C9-C8
3	A	1298	LDA	C2-C3-C4-C5
3	B	1307	LDA	C6-C7-C8-C9
3	B	1323	LDA	C2-C3-C4-C5
3	C	1327	LDA	C11-C10-C9-C8
3	A	1293	LDA	C3-C4-C5-C6
3	A	1295	LDA	C6-C7-C8-C9
3	A	1311	LDA	C11-C10-C9-C8
3	A	1321	LDA	C5-C6-C7-C8
3	A	1322	LDA	C2-C3-C4-C5
3	A	1326	LDA	C6-C7-C8-C9
3	B	1298	LDA	C5-C6-C7-C8
3	B	1317	LDA	C2-C3-C4-C5
3	B	1317	LDA	C3-C4-C5-C6
3	C	1297	LDA	C5-C6-C7-C8
3	D	1294	LDA	C3-C4-C5-C6
3	A	1313	LDA	C4-C5-C6-C7
3	B	1313	LDA	C3-C4-C5-C6
3	B	1318	LDA	C2-C3-C4-C5
3	C	1293	LDA	C3-C4-C5-C6
3	D	1298	LDA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	A	1297	LDA	C5-C6-C7-C8
3	A	1316	LDA	C11-C10-C9-C8
3	B	1291	LDA	C7-C8-C9-C10
3	B	1327	LDA	C5-C6-C7-C8
3	B	1329	LDA	C7-C8-C9-C10
3	C	1315	LDA	C2-C3-C4-C5
3	D	1290	LDA	C6-C7-C8-C9
3	A	1306	LDA	C6-C7-C8-C9
3	A	1327	LDA	C6-C7-C8-C9
3	B	1297	LDA	C11-C10-C9-C8
3	B	1308	LDA	C11-C10-C9-C8
3	B	1311	LDA	C5-C6-C7-C8
3	B	1318	LDA	C6-C7-C8-C9
3	B	1329	LDA	C3-C4-C5-C6
3	C	1290	LDA	C7-C8-C9-C10
3	C	1291	LDA	C11-C10-C9-C8
3	C	1313	LDA	C6-C7-C8-C9
3	D	1290	LDA	C4-C5-C6-C7
3	D	1296	LDA	C6-C7-C8-C9
3	D	1299	LDA	C2-C3-C4-C5
3	A	1310	LDA	C11-C10-C9-C8
3	B	1298	LDA	C6-C7-C8-C9
3	B	1303	LDA	C6-C7-C8-C9
3	D	1291	LDA	C7-C8-C9-C10
3	D	1297	LDA	C11-C10-C9-C8
3	A	1296	LDA	C11-C10-C9-C8
3	A	1302	LDA	C6-C7-C8-C9
3	A	1320	LDA	C5-C6-C7-C8
3	D	1303	LDA	C6-C7-C8-C9
3	A	1314	LDA	C2-C3-C4-C5
3	A	1320	LDA	C6-C7-C8-C9
3	B	1295	LDA	C5-C6-C7-C8
3	B	1315	LDA	C3-C4-C5-C6
3	B	1319	LDA	C5-C6-C7-C8
3	B	1329	LDA	C6-C7-C8-C9
3	C	1295	LDA	C6-C7-C8-C9
3	C	1302	LDA	C6-C7-C8-C9
3	C	1304	LDA	C6-C7-C8-C9
3	C	1309	LDA	C4-C5-C6-C7
3	C	1315	LDA	C5-C6-C7-C8
3	D	1306	LDA	C2-C3-C4-C5
3	D	1309	LDA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	A	413	LDA	C9-C10-C11-C12
3	A	1289	LDA	C6-C7-C8-C9
3	A	1320	LDA	C3-C4-C5-C6
3	B	1313	LDA	C5-C6-C7-C8
3	B	1314	LDA	C6-C7-C8-C9
3	C	1308	LDA	C2-C3-C4-C5
3	C	1321	LDA	C4-C5-C6-C7
3	A	1290	LDA	C7-C8-C9-C10
3	A	1323	LDA	C3-C4-C5-C6
3	B	1309	LDA	C4-C5-C6-C7
3	B	1325	LDA	C4-C5-C6-C7
3	C	1296	LDA	C11-C10-C9-C8
3	C	1310	LDA	C6-C7-C8-C9
3	A	1316	LDA	C7-C8-C9-C10
3	B	1301	LDA	C6-C7-C8-C9
3	B	1317	LDA	C5-C6-C7-C8
3	C	1325	LDA	C5-C6-C7-C8
3	C	1327	LDA	C3-C4-C5-C6
3	C	413	LDA	C9-C10-C11-C12
3	C	1295	LDA	C11-C10-C9-C8
3	A	1289	LDA	C1-C2-C3-C4
3	B	1304	LDA	C1-C2-C3-C4
3	B	1313	LDA	C1-C2-C3-C4
3	D	1304	LDA	C1-C2-C3-C4
3	A	413	LDA	C3-C4-C5-C6
3	A	1300	LDA	C4-C5-C6-C7
3	B	1290	LDA	C4-C5-C6-C7
3	B	1325	LDA	C7-C8-C9-C10
3	C	1326	LDA	C7-C8-C9-C10
3	A	1325	LDA	C9-C10-C11-C12
3	B	413	LDA	C9-C10-C11-C12
3	C	1298	LDA	C9-C10-C11-C12
3	B	1304	LDA	C7-C8-C9-C10
3	C	1315	LDA	C4-C5-C6-C7
3	C	1321	LDA	C2-C3-C4-C5
3	B	1316	LDA	C1-C2-C3-C4
3	D	1313	LDA	C1-C2-C3-C4
3	B	1290	LDA	C6-C7-C8-C9
3	C	413	LDA	C3-C4-C5-C6
3	C	1289	LDA	C6-C7-C8-C9
3	C	1318	LDA	C7-C8-C9-C10
3	C	1281	LDA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	C	1315	LDA	C11-C10-C9-C8
3	B	1329	LDA	C1-C2-C3-C4
3	D	1290	LDA	C1-C2-C3-C4
3	A	1313	LDA	C3-C4-C5-C6
3	A	1322	LDA	C6-C7-C8-C9
3	A	1325	LDA	C3-C4-C5-C6
3	B	1300	LDA	C7-C8-C9-C10
3	B	1318	LDA	C3-C4-C5-C6
3	C	1289	LDA	C4-C5-C6-C7
3	C	1295	LDA	C2-C3-C4-C5
3	D	1301	LDA	C11-C10-C9-C8
3	A	1295	LDA	C2-C3-C4-C5
3	A	1324	LDA	C2-C3-C4-C5
3	C	1299	LDA	C7-C8-C9-C10
3	C	1314	LDA	C3-C4-C5-C6
3	D	1297	LDA	C5-C6-C7-C8
3	B	1327	LDA	C1-C2-C3-C4
3	A	1302	LDA	C11-C10-C9-C8
3	A	1319	LDA	C3-C4-C5-C6
3	B	1296	LDA	C2-C3-C4-C5
3	C	1316	LDA	C3-C4-C5-C6
3	D	1296	LDA	C2-C3-C4-C5
3	A	1307	LDA	C1-C2-C3-C4
3	B	1323	LDA	C3-C4-C5-C6
3	C	1328	LDA	C3-C4-C5-C6
3	A	1299	LDA	C7-C8-C9-C10
3	B	413	LDA	C3-C4-C5-C6
3	B	1296	LDA	C11-C10-C9-C8
3	C	1291	LDA	C6-C7-C8-C9
3	C	1296	LDA	C5-C6-C7-C8
3	C	1302	LDA	C11-C10-C9-C8
3	C	1321	LDA	C5-C6-C7-C8
3	D	1296	LDA	C11-C10-C9-C8
3	D	1299	LDA	C9-C10-C11-C12
3	B	1290	LDA	C1-C2-C3-C4
3	C	1327	LDA	C1-C2-C3-C4
3	A	1298	LDA	C9-C10-C11-C12
3	A	1327	LDA	C5-C6-C7-C8
3	B	1297	LDA	C5-C6-C7-C8
3	A	1291	LDA	C4-C5-C6-C7
3	A	1304	LDA	C7-C8-C9-C10
3	A	1306	LDA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
3	B	1307	LDA	C11-C10-C9-C8
3	B	1324	LDA	C5-C6-C7-C8
3	C	1291	LDA	C4-C5-C6-C7
3	B	1299	LDA	C9-C10-C11-C12
3	A	1319	LDA	C1-C2-C3-C4
3	C	1307	LDA	C2-C3-C4-C5
3	A	1304	LDA	C1-C2-C3-C4
3	A	1308	LDA	C1-C2-C3-C4
3	C	1311	LDA	C2-C3-C4-C5
3	D	1300	LDA	C7-C8-C9-C10
3	D	1308	LDA	C1-C2-C3-C4
3	A	1295	LDA	C11-C10-C9-C8
3	A	1300	LDA	C3-C4-C5-C6
3	A	1300	LDA	C5-C6-C7-C8
3	A	1315	LDA	C1-C2-C3-C4
3	C	1323	LDA	C1-C2-C3-C4
3	A	1312	LDA	C2-C3-C4-C5
3	A	1326	LDA	C11-C10-C9-C8
3	C	1294	LDA	C5-C6-C7-C8
3	C	1312	LDA	C5-C6-C7-C8
3	D	1300	LDA	C6-C7-C8-C9
3	D	1291	LDA	C6-C7-C8-C9
3	D	1303	LDA	C11-C10-C9-C8
3	B	1301	LDA	C1-C2-C3-C4
3	C	1307	LDA	C1-C2-C3-C4
3	C	1318	LDA	C1-C2-C3-C4
3	A	1303	LDA	C6-C7-C8-C9
3	B	1311	LDA	C11-C10-C9-C8
3	A	1289	LDA	C4-C5-C6-C7
3	B	1292	LDA	C6-C7-C8-C9
3	C	1318	LDA	C5-C6-C7-C8
3	D	1292	LDA	C4-C5-C6-C7
3	D	1292	LDA	C6-C7-C8-C9
3	B	1324	LDA	C3-C4-C5-C6
3	B	1328	LDA	C6-C7-C8-C9
3	B	1320	LDA	C4-C5-C6-C7
3	B	1324	LDA	C7-C8-C9-C10
3	C	1314	LDA	C11-C10-C9-C8
3	B	1325	LDA	C1-C2-C3-C4
3	C	1289	LDA	C1-C2-C3-C4
3	A	1296	LDA	C5-C6-C7-C8
3	A	1324	LDA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	B	1311	LDA	C4-C5-C6-C7
3	D	1308	LDA	C2-C3-C4-C5
3	B	1300	LDA	C6-C7-C8-C9
3	B	1303	LDA	C11-C10-C9-C8
3	C	1322	LDA	C4-C5-C6-C7
3	C	1326	LDA	C1-C2-C3-C4
3	C	1327	LDA	C2-C3-C4-C5
3	D	1299	LDA	C1-C2-C3-C4
3	A	1313	LDA	C6-C7-C8-C9
3	B	1310	LDA	C4-C5-C6-C7
3	B	1313	LDA	C11-C10-C9-C8
3	C	1304	LDA	C11-C10-C9-C8
3	C	1317	LDA	C4-C5-C6-C7
3	B	1307	LDA	C1-C2-C3-C4
3	A	1028	LDA	C2-C3-C4-C5
3	B	1292	LDA	C3-C4-C5-C6
3	B	1315	LDA	C4-C5-C6-C7
3	C	1281	LDA	C6-C7-C8-C9
3	C	1299	LDA	C6-C7-C8-C9
3	C	1321	LDA	C11-C10-C9-C8
3	C	1326	LDA	C5-C6-C7-C8
3	A	1291	LDA	C6-C7-C8-C9
3	A	1294	LDA	C5-C6-C7-C8
3	A	1323	LDA	C6-C7-C8-C9
3	B	1322	LDA	C5-C6-C7-C8
3	B	1329	LDA	C11-C10-C9-C8
3	C	1323	LDA	C2-C3-C4-C5
3	D	1293	LDA	C4-C5-C6-C7
3	A	1322	LDA	C5-C6-C7-C8
3	B	1292	LDA	C4-C5-C6-C7
3	B	1293	LDA	C4-C5-C6-C7
3	B	1300	LDA	C11-C10-C9-C8
3	B	1322	LDA	C4-C5-C6-C7
3	C	1290	LDA	C6-C7-C8-C9
3	D	1300	LDA	C11-C10-C9-C8
3	D	1309	LDA	C7-C8-C9-C10
3	B	1299	LDA	C1-C2-C3-C4
3	A	1292	LDA	C4-C5-C6-C7
3	A	1295	LDA	C7-C8-C9-C10
3	A	1324	LDA	C4-C5-C6-C7
3	C	1295	LDA	C7-C8-C9-C10
3	D	1301	LDA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	1291	LDA	C3-C4-C5-C6
3	B	1328	LDA	C2-C3-C4-C5
3	C	1299	LDA	C11-C10-C9-C8
3	C	1306	LDA	C6-C7-C8-C9
3	C	1321	LDA	C6-C7-C8-C9
3	A	1298	LDA	C1-C2-C3-C4
3	A	1318	LDA	C1-C2-C3-C4
3	B	1311	LDA	C1-C2-C3-C4
3	C	1298	LDA	C1-C2-C3-C4
3	C	1312	LDA	C1-C2-C3-C4
3	A	1314	LDA	C1-C2-C3-C4
3	A	1028	LDA	C6-C7-C8-C9
3	B	1291	LDA	C6-C7-C8-C9
3	C	1291	LDA	C3-C4-C5-C6
3	D	1292	LDA	C3-C4-C5-C6
3	D	1306	LDA	C4-C5-C6-C7
3	A	1299	LDA	C6-C7-C8-C9
3	A	1299	LDA	C11-C10-C9-C8
3	C	1292	LDA	C4-C5-C6-C7
3	C	1318	LDA	C2-C3-C4-C5
3	A	1290	LDA	C6-C7-C8-C9
3	A	1303	LDA	C2-C3-C4-C5
3	D	1296	LDA	C7-C8-C9-C10
3	A	1309	LDA	C11-C10-C9-C8
3	B	1314	LDA	C7-C8-C9-C10
3	D	1310	LDA	C4-C5-C6-C7
3	A	1292	LDA	C1-C2-C3-C4
3	D	1293	LDA	C1-C2-C3-C4
3	A	1318	LDA	C11-C10-C9-C8
3	B	1296	LDA	C7-C8-C9-C10
3	B	1316	LDA	C4-C5-C6-C7
3	B	1293	LDA	C1-C2-C3-C4
3	B	1323	LDA	C1-C2-C3-C4
3	A	1300	LDA	C6-C7-C8-C9
3	C	1316	LDA	C6-C7-C8-C9
3	D	1292	LDA	C7-C8-C9-C10
3	C	1289	LDA	C5-C6-C7-C8
3	D	1313	LDA	C11-C10-C9-C8
3	B	1290	LDA	C5-C6-C7-C8
3	A	1320	LDA	C1-C2-C3-C4
3	A	1289	LDA	C11-C10-C9-C8
3	C	1300	LDA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	D	1309	LDA	C4-C5-C6-C7
3	A	1308	LDA	C2-C3-C4-C5
3	C	1296	LDA	C3-C4-C5-C6
3	D	1290	LDA	C11-C10-C9-C8
3	B	1306	LDA	C1-C2-C3-C4
3	C	1292	LDA	C1-C2-C3-C4
3	A	1292	LDA	C11-C10-C9-C8
3	A	1315	LDA	C2-C3-C4-C5
3	B	1290	LDA	C11-C10-C9-C8
3	A	1309	LDA	C1-C2-C3-C4
3	C	1321	LDA	C1-C2-C3-C4
3	C	1309	LDA	C2-C3-C4-C5
3	B	1304	LDA	C6-C7-C8-C9
3	C	1281	LDA	C2-C3-C4-C5
3	A	1289	LDA	C5-C6-C7-C8
3	B	1310	LDA	C3-C4-C5-C6
3	C	1293	LDA	C7-C8-C9-C10
3	A	1028	LDA	C1-C2-C3-C4
3	B	1319	LDA	C1-C2-C3-C4
3	C	1293	LDA	C1-C2-C3-C4
3	D	1308	LDA	C7-C8-C9-C10
3	D	1309	LDA	C1-C2-C3-C4
3	A	1309	LDA	C2-C3-C4-C5
3	A	1321	LDA	C6-C7-C8-C9
3	C	1281	LDA	C4-C5-C6-C7
3	C	1289	LDA	C11-C10-C9-C8
3	C	1306	LDA	C3-C4-C5-C6
3	D	1311	LDA	C5-C6-C7-C8
3	D	1295	LDA	C5-C6-C7-C8
3	D	1307	LDA	C2-C3-C4-C5
3	A	1310	LDA	C1-C2-C3-C4
3	B	1323	LDA	C5-C6-C7-C8
3	C	1315	LDA	C1-C2-C3-C4
3	A	1315	LDA	C6-C7-C8-C9
3	B	1297	LDA	C3-C4-C5-C6
3	D	1281	LDA	C3-C4-C5-C6
3	D	1291	LDA	C1-C2-C3-C4
3	B	1292	LDA	C7-C8-C9-C10
3	B	1293	LDA	C11-C10-C9-C8
3	D	1290	LDA	C5-C6-C7-C8
3	D	1297	LDA	C3-C4-C5-C6
3	A	1305	LDA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	C	1316	LDA	C7-C8-C9-C10
3	B	1330	LDA	C6-C7-C8-C9
3	D	1307	LDA	C11-C10-C9-C8
3	B	1329	LDA	C4-C5-C6-C7
3	A	1320	LDA	C7-C8-C9-C10
3	C	1325	LDA	C4-C5-C6-C7
3	C	1303	LDA	C1-C2-C3-C4
3	A	1296	LDA	C3-C4-C5-C6
3	A	1303	LDA	C11-C10-C9-C8
3	C	1291	LDA	C7-C8-C9-C10
3	D	1293	LDA	C11-C10-C9-C8
3	D	1313	LDA	C2-C3-C4-C5
3	B	1317	LDA	C1-C2-C3-C4
3	D	1307	LDA	C1-C2-C3-C4
3	A	1314	LDA	C4-C5-C6-C7
3	B	1305	LDA	C6-C7-C8-C9
3	B	1326	LDA	C4-C5-C6-C7
3	C	1316	LDA	C5-C6-C7-C8
3	C	1322	LDA	C3-C4-C5-C6
3	D	1294	LDA	C7-C8-C9-C10
3	C	1301	LDA	C3-C4-C5-C6
3	D	1281	LDA	C6-C7-C8-C9
3	A	1293	LDA	C1-C2-C3-C4
3	D	1294	LDA	C1-C2-C3-C4
3	B	1306	LDA	C11-C10-C9-C8
3	D	1308	LDA	C4-C5-C6-C7
3	B	1329	LDA	C9-C10-C11-C12
3	C	1322	LDA	C1-C2-C3-C4
3	A	1304	LDA	C6-C7-C8-C9
3	D	1281	LDA	C5-C6-C7-C8
3	A	1305	LDA	C1-C2-C3-C4
3	B	1305	LDA	C1-C2-C3-C4
3	A	1291	LDA	C7-C8-C9-C10
3	B	1294	LDA	C7-C8-C9-C10
3	D	1282	LDA	C1-C2-C3-C4
3	B	1302	LDA	C3-C4-C5-C6
3	C	1316	LDA	C4-C5-C6-C7
3	D	1308	LDA	C6-C7-C8-C9
3	A	1300	LDA	C9-C10-C11-C12
3	A	1293	LDA	C7-C8-C9-C10
3	C	1292	LDA	C11-C10-C9-C8
3	A	1317	LDA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	A	1301	LDA	C3-C4-C5-C6
3	B	1310	LDA	C5-C6-C7-C8
3	B	1328	LDA	C4-C5-C6-C7
3	D	1305	LDA	C3-C4-C5-C6
3	A	1307	LDA	C9-C10-C11-C12
3	A	1307	LDA	N1-C1-C2-C3
3	B	1318	LDA	N1-C1-C2-C3
3	B	1322	LDA	N1-C1-C2-C3
3	C	1305	LDA	N1-C1-C2-C3
3	D	1282	LDA	N1-C1-C2-C3
3	D	1304	LDA	N1-C1-C2-C3
3	B	1301	LDA	C3-C4-C5-C6
3	B	1306	LDA	C2-C3-C4-C5
3	D	1302	LDA	C3-C4-C5-C6
3	D	1309	LDA	C6-C7-C8-C9
3	B	1315	LDA	C9-C10-C11-C12
3	D	1304	LDA	C9-C10-C11-C12
3	A	1300	LDA	C11-C10-C9-C8
3	B	1296	LDA	C5-C6-C7-C8
3	A	1290	LDA	C1-C2-C3-C4
3	A	1324	LDA	C9-C10-C11-C12
3	A	1318	LDA	C5-C6-C7-C8
3	B	1318	LDA	C11-C10-C9-C8
3	A	1295	LDA	C5-C6-C7-C8
3	B	1306	LDA	C5-C6-C7-C8
3	B	1328	LDA	C9-C10-C11-C12
3	C	1328	LDA	C9-C10-C11-C12
3	A	1309	LDA	C5-C6-C7-C8
3	B	1328	LDA	C11-C10-C9-C8
3	B	1319	LDA	C6-C7-C8-C9
3	B	1330	LDA	C3-C4-C5-C6
3	A	1318	LDA	C9-C10-C11-C12
3	C	1303	LDA	C6-C7-C8-C9
3	A	1323	LDA	C9-C10-C11-C12
3	D	1282	LDA	C9-C10-C11-C12
3	B	1294	LDA	C1-C2-C3-C4
3	B	1301	LDA	C4-C5-C6-C7
3	B	1304	LDA	C9-C10-C11-C12
3	B	1305	LDA	C7-C8-C9-C10
3	B	1322	LDA	C3-C4-C5-C6
3	D	1296	LDA	C5-C6-C7-C8
3	D	1305	LDA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	C	1315	LDA	C3-C4-C5-C6
3	D	1292	LDA	C5-C6-C7-C8
3	A	1314	LDA	C6-C7-C8-C9
3	A	1326	LDA	C4-C5-C6-C7
3	C	1305	LDA	C1-C2-C3-C4
3	A	1300	LDA	C2-C3-C4-C5
3	B	1317	LDA	C11-C10-C9-C8
3	C	1300	LDA	C3-C4-C5-C6
3	C	1304	LDA	C4-C5-C6-C7
3	D	1298	LDA	C2-C3-C4-C5
3	D	1305	LDA	C5-C6-C7-C8
3	A	1304	LDA	C9-C10-C11-C12
3	A	1028	LDA	C5-C6-C7-C8
3	B	1292	LDA	C5-C6-C7-C8
3	B	1325	LDA	C5-C6-C7-C8
3	D	1307	LDA	C5-C6-C7-C8
3	C	1313	LDA	C9-C10-C11-C12
3	C	1312	LDA	C9-C10-C11-C12
3	A	1303	LDA	C4-C5-C6-C7
3	A	1305	LDA	C7-C8-C9-C10
3	A	1291	LDA	C5-C6-C7-C8
3	A	1303	LDA	C9-C10-C11-C12
3	A	1311	LDA	C2-C3-C4-C5
3	C	1320	LDA	C6-C7-C8-C9
3	A	1289	LDA	C9-C10-C11-C12
3	B	1302	LDA	C2-C3-C4-C5
3	A	1311	LDA	C5-C6-C7-C8
3	B	1290	LDA	C9-C10-C11-C12
3	C	1313	LDA	C7-C8-C9-C10
3	D	1290	LDA	C9-C10-C11-C12
3	C	1317	LDA	C11-C10-C9-C8
3	D	1281	LDA	C1-C2-C3-C4
3	C	1297	LDA	C2-C3-C4-C5
3	C	1306	LDA	C5-C6-C7-C8
3	A	1302	LDA	C7-C8-C9-C10
3	B	1325	LDA	C11-C10-C9-C8
3	C	1289	LDA	C9-C10-C11-C12
3	A	1028	LDA	C3-C4-C5-C6
3	C	1295	LDA	C5-C6-C7-C8
3	C	1308	LDA	C3-C4-C5-C6
3	C	1319	LDA	C3-C4-C5-C6
3	A	1324	LDA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	C	1317	LDA	C1-C2-C3-C4
3	D	1301	LDA	C9-C10-C11-C12
3	C	1317	LDA	C3-C4-C5-C6
3	C	1309	LDA	C5-C6-C7-C8
3	D	1282	LDA	C6-C7-C8-C9
3	B	1303	LDA	C7-C8-C9-C10
3	B	1311	LDA	C7-C8-C9-C10
3	B	1314	LDA	C9-C10-C11-C12
3	C	1308	LDA	C1-C2-C3-C4
3	C	1300	LDA	C5-C6-C7-C8
3	A	1313	LDA	C2-C3-C4-C5
3	C	1302	LDA	C7-C8-C9-C10
3	A	1321	LDA	C2-C3-C4-C5
3	A	1322	LDA	C11-C10-C9-C8
3	A	1323	LDA	C11-C10-C9-C8
3	B	1298	LDA	C2-C3-C4-C5
3	C	1312	LDA	C6-C7-C8-C9
3	D	1304	LDA	C7-C8-C9-C10
3	A	1306	LDA	C4-C5-C6-C7
3	C	1301	LDA	C2-C3-C4-C5
3	D	1302	LDA	C2-C3-C4-C5
3	A	1307	LDA	C7-C8-C9-C10
3	C	1281	LDA	C3-C4-C5-C6
3	C	1291	LDA	C5-C6-C7-C8
3	C	1306	LDA	C7-C8-C9-C10
3	D	1311	LDA	C4-C5-C6-C7
3	C	1290	LDA	C1-C2-C3-C4
3	D	1311	LDA	C9-C10-C11-C12
3	A	1302	LDA	C1-C2-C3-C4
3	B	1294	LDA	C9-C10-C11-C12
3	B	1315	LDA	C7-C8-C9-C10
3	B	1320	LDA	C7-C8-C9-C10
3	C	1316	LDA	C2-C3-C4-C5
3	C	1319	LDA	C11-C10-C9-C8
3	A	1315	LDA	C4-C5-C6-C7
3	B	1300	LDA	C2-C3-C4-C5
3	D	1301	LDA	C6-C7-C8-C9
3	B	1301	LDA	C2-C3-C4-C5
3	B	1312	LDA	C4-C5-C6-C7
3	D	1310	LDA	C11-C10-C9-C8
3	C	1320	LDA	C1-C2-C3-C4
3	D	1305	LDA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	A	1312	LDA	C11-C10-C9-C8
3	D	1303	LDA	C7-C8-C9-C10
3	D	1292	LDA	C2-C3-C4-C5
3	D	1294	LDA	C9-C10-C11-C12
3	B	1303	LDA	C9-C10-C11-C12
3	C	1293	LDA	C9-C10-C11-C12
3	C	1302	LDA	C1-C2-C3-C4
3	C	1306	LDA	C1-C2-C3-C4
3	A	1293	LDA	C9-C10-C11-C12
3	C	1325	LDA	C7-C8-C9-C10
3	C	1324	LDA	C9-C10-C11-C12
3	B	1303	LDA	C1-C2-C3-C4
3	B	1308	LDA	C1-C2-C3-C4
3	B	1327	LDA	C2-C3-C4-C5
3	C	1320	LDA	C2-C3-C4-C5
3	C	1319	LDA	C2-C3-C4-C5
3	D	1303	LDA	C1-C2-C3-C4
3	D	1293	LDA	C9-C10-C11-C12
3	C	1299	LDA	C2-C3-C4-C5
3	B	1320	LDA	C9-C10-C11-C12
3	C	1292	LDA	C9-C10-C11-C12
3	B	1321	LDA	C2-C3-C4-C5
3	D	1311	LDA	C6-C7-C8-C9
3	A	1299	LDA	C2-C3-C4-C5
3	A	1301	LDA	C2-C3-C4-C5
3	A	1304	LDA	C5-C6-C7-C8
3	C	1291	LDA	C2-C3-C4-C5
3	B	1293	LDA	C9-C10-C11-C12
3	B	1323	LDA	C9-C10-C11-C12
3	A	1315	LDA	C7-C8-C9-C10
3	A	1315	LDA	C9-C10-C11-C12
3	B	1296	LDA	C9-C10-C11-C12
3	B	1291	LDA	C1-C2-C3-C4
3	B	482	LDA	C9-C10-C11-C12
3	C	1302	LDA	C9-C10-C11-C12
3	D	1296	LDA	C9-C10-C11-C12
3	A	1291	LDA	C2-C3-C4-C5
3	D	1311	LDA	C11-C10-C9-C8
3	C	1299	LDA	C3-C4-C5-C6
3	A	1296	LDA	C9-C10-C11-C12
3	B	1304	LDA	C5-C6-C7-C8
3	A	1292	LDA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	C	1295	LDA	C9-C10-C11-C12
3	B	1314	LDA	C5-C6-C7-C8
3	B	1330	LDA	C11-C10-C9-C8
3	B	1300	LDA	C3-C4-C5-C6
3	B	1310	LDA	C11-C10-C9-C8
3	C	1317	LDA	C6-C7-C8-C9
3	D	1281	LDA	C7-C8-C9-C10
3	C	1319	LDA	C9-C10-C11-C12
4	B	1289	TAM	C-C1-C4-O4
3	B	1323	LDA	C6-C7-C8-C9
3	A	1299	LDA	C3-C4-C5-C6
3	D	1313	LDA	C5-C6-C7-C8
3	C	1310	LDA	C11-C10-C9-C8
3	A	1308	LDA	C9-C10-C11-C12
3	C	1309	LDA	C7-C8-C9-C10
3	D	1303	LDA	C9-C10-C11-C12
3	C	1315	LDA	C7-C8-C9-C10
3	B	482	LDA	C1-C2-C3-C4
3	C	1305	LDA	C3-C4-C5-C6
3	B	1292	LDA	C2-C3-C4-C5
3	C	1296	LDA	C9-C10-C11-C12
3	D	1300	LDA	C2-C3-C4-C5
3	D	1305	LDA	C7-C8-C9-C10
3	B	1308	LDA	C4-C5-C6-C7
3	C	1296	LDA	C2-C3-C4-C5
3	C	1303	LDA	C7-C8-C9-C10
3	A	1295	LDA	C9-C10-C11-C12
3	C	1322	LDA	C5-C6-C7-C8
3	A	1327	LDA	C11-C10-C9-C8
3	B	1297	LDA	C9-C10-C11-C12
3	D	1308	LDA	C9-C10-C11-C12
3	A	1301	LDA	C2-C1-N1-CM1
3	A	1309	LDA	C2-C1-N1-CM1
3	A	1309	LDA	C2-C1-N1-CM2
3	A	1310	LDA	C2-C1-N1-CM1
3	A	1311	LDA	C2-C1-N1-CM1
3	A	1311	LDA	C2-C1-N1-CM2
3	A	1312	LDA	C2-C1-N1-CM1
3	A	1312	LDA	C2-C1-N1-CM2
3	A	1316	LDA	C2-C1-N1-CM1
3	A	1320	LDA	C2-C1-N1-CM1
3	A	1324	LDA	C2-C1-N1-CM1

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Mol	Chain	Res	Type	Atoms
3	A	1324	LDA	C2-C1-N1-CM2
3	B	1302	LDA	C2-C1-N1-CM1
3	B	1306	LDA	C2-C1-N1-CM1
3	B	1306	LDA	C2-C1-N1-CM2
3	B	1307	LDA	C2-C1-N1-CM1
3	B	1308	LDA	C2-C1-N1-CM1
3	B	1308	LDA	C2-C1-N1-CM2
3	B	1309	LDA	C2-C1-N1-CM1
3	B	1316	LDA	C2-C1-N1-CM1
3	B	1317	LDA	C2-C1-N1-CM1
3	B	1318	LDA	C2-C1-N1-CM2
3	B	1320	LDA	C2-C1-N1-CM1
3	B	1321	LDA	C2-C1-N1-CM1
3	B	1323	LDA	C2-C1-N1-CM2
3	B	1324	LDA	C2-C1-N1-CM1
3	B	1326	LDA	C2-C1-N1-CM1
3	C	1281	LDA	C2-C1-N1-CM1
3	C	1301	LDA	C2-C1-N1-CM1
3	C	1307	LDA	C2-C1-N1-CM2
3	C	1311	LDA	C2-C1-N1-CM1
3	C	1311	LDA	C2-C1-N1-CM2
3	C	1321	LDA	C2-C1-N1-CM1
3	C	1322	LDA	C2-C1-N1-CM1
3	C	1323	LDA	C2-C1-N1-CM1
3	C	1326	LDA	C2-C1-N1-CM1
3	C	1327	LDA	C2-C1-N1-CM1
3	D	1302	LDA	C2-C1-N1-CM1
3	D	1306	LDA	C2-C1-N1-CM2
3	D	1307	LDA	C2-C1-N1-CM1
3	D	1307	LDA	C2-C1-N1-CM2
3	D	1309	LDA	C2-C1-N1-CM1
3	D	1311	LDA	C2-C1-N1-CM1
3	D	1311	LDA	C2-C1-N1-CM2
3	A	1314	LDA	C5-C6-C7-C8
3	D	1313	LDA	C6-C7-C8-C9
3	A	1302	LDA	C9-C10-C11-C12
3	A	1297	LDA	C2-C3-C4-C5
3	D	1311	LDA	C2-C3-C4-C5
3	D	1307	LDA	C4-C5-C6-C7
3	B	1306	LDA	C4-C5-C6-C7
3	A	1296	LDA	C2-C3-C4-C5
3	B	1315	LDA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	B	1318	LDA	C9-C10-C11-C12
3	C	1305	LDA	C2-C3-C4-C5
3	D	1311	LDA	C7-C8-C9-C10
3	C	1318	LDA	C11-C10-C9-C8
3	B	482	LDA	C6-C7-C8-C9
3	B	1327	LDA	C9-C10-C11-C12
3	D	1313	LDA	C7-C8-C9-C10
3	A	1305	LDA	C5-C6-C7-C8
3	A	1309	LDA	C4-C5-C6-C7
3	B	1321	LDA	C11-C10-C9-C8
3	A	1028	LDA	C2-C1-N1-O1
3	A	1294	LDA	C2-C1-N1-O1
3	A	1307	LDA	C2-C1-N1-O1
3	A	1309	LDA	C2-C1-N1-O1
3	A	1311	LDA	C2-C1-N1-O1
3	A	1312	LDA	C2-C1-N1-O1
3	A	1323	LDA	C2-C1-N1-O1
3	A	1324	LDA	C2-C1-N1-O1
3	B	1295	LDA	C2-C1-N1-O1
3	B	1306	LDA	C2-C1-N1-O1
3	B	1308	LDA	C2-C1-N1-O1
3	B	1309	LDA	C2-C1-N1-O1
3	B	1312	LDA	C2-C1-N1-O1
3	B	1314	LDA	C2-C1-N1-O1
3	B	1315	LDA	C2-C1-N1-O1
3	B	1317	LDA	C2-C1-N1-O1
3	B	1321	LDA	C2-C1-N1-O1
3	B	1326	LDA	C2-C1-N1-O1
3	C	1281	LDA	C2-C1-N1-O1
3	C	1294	LDA	C2-C1-N1-O1
3	C	1305	LDA	C2-C1-N1-O1
3	C	1307	LDA	C2-C1-N1-O1
3	C	1308	LDA	C2-C1-N1-O1
3	C	1311	LDA	C2-C1-N1-O1
3	C	1313	LDA	C2-C1-N1-O1
3	C	1319	LDA	C2-C1-N1-O1
3	C	1320	LDA	C2-C1-N1-O1
3	D	1302	LDA	C2-C1-N1-O1
3	D	1304	LDA	C2-C1-N1-O1
3	D	1307	LDA	C2-C1-N1-O1
3	D	1311	LDA	C2-C1-N1-O1
3	A	1313	LDA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
3	D	1297	LDA	C2-C3-C4-C5
3	C	1291	LDA	C9-C10-C11-C12
3	A	1321	LDA	C9-C10-C11-C12
3	B	1304	LDA	C2-C3-C4-C5
3	C	1300	LDA	C4-C5-C6-C7
3	C	1319	LDA	C6-C7-C8-C9
3	D	1309	LDA	C9-C10-C11-C12
3	D	1297	LDA	C9-C10-C11-C12
3	B	1309	LDA	C2-C3-C4-C5
3	D	1281	LDA	C4-C5-C6-C7
3	C	1328	LDA	C2-C3-C4-C5
3	A	1297	LDA	C9-C10-C11-C12
3	D	1292	LDA	C9-C10-C11-C12
3	A	1322	LDA	C3-C4-C5-C6
3	D	1301	LDA	C1-C2-C3-C4
3	B	1320	LDA	C11-C10-C9-C8
3	A	1313	LDA	C7-C8-C9-C10
3	A	1317	LDA	C3-C4-C5-C6
3	C	1323	LDA	C5-C6-C7-C8
3	C	1313	LDA	C1-C2-C3-C4
3	A	1327	LDA	C4-C5-C6-C7
3	A	1297	LDA	C3-C4-C5-C6
3	B	1311	LDA	C2-C3-C4-C5
3	A	1317	LDA	C4-C5-C6-C7
3	A	1327	LDA	C3-C4-C5-C6
3	B	1314	LDA	C1-C2-C3-C4
3	C	1308	LDA	C9-C10-C11-C12
3	C	1311	LDA	C5-C6-C7-C8
3	A	1307	LDA	C5-C6-C7-C8
3	C	1310	LDA	C5-C6-C7-C8
3	C	1324	LDA	C2-C3-C4-C5
3	B	1292	LDA	C9-C10-C11-C12
3	D	1305	LDA	C4-C5-C6-C7
3	B	1324	LDA	C11-C10-C9-C8
3	C	1294	LDA	C9-C10-C11-C12
3	A	1304	LDA	C2-C3-C4-C5
3	C	413	LDA	C7-C8-C9-C10
3	D	1306	LDA	C9-C10-C11-C12
3	B	1308	LDA	C2-C3-C4-C5
3	B	1326	LDA	C7-C8-C9-C10
3	A	1305	LDA	C11-C10-C9-C8
3	D	1302	LDA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	A	1310	LDA	N1-C1-C2-C3
3	A	1315	LDA	N1-C1-C2-C3
3	A	1317	LDA	N1-C1-C2-C3
3	B	482	LDA	N1-C1-C2-C3
3	B	1307	LDA	N1-C1-C2-C3
3	B	1314	LDA	N1-C1-C2-C3
3	B	1330	LDA	N1-C1-C2-C3
3	C	1310	LDA	N1-C1-C2-C3
3	C	1326	LDA	N1-C1-C2-C3
3	C	1325	LDA	C1-C2-C3-C4
3	B	1297	LDA	C2-C3-C4-C5
3	A	413	LDA	C7-C8-C9-C10
3	D	1310	LDA	C1-C2-C3-C4
3	B	413	LDA	C7-C8-C9-C10
3	A	1316	LDA	C5-C6-C7-C8
3	A	1301	LDA	C9-C10-C11-C12
3	B	482	LDA	C4-C5-C6-C7
3	D	1305	LDA	C9-C10-C11-C12
3	C	1325	LDA	C3-C4-C5-C6
3	D	1304	LDA	C5-C6-C7-C8
3	A	1311	LDA	C1-C2-C3-C4
3	C	1301	LDA	C9-C10-C11-C12
3	B	1321	LDA	C3-C4-C5-C6
3	C	1324	LDA	C11-C10-C9-C8
3	B	1293	LDA	C3-C4-C5-C6
3	A	1291	LDA	C9-C10-C11-C12
3	C	1317	LDA	C5-C6-C7-C8
3	B	1310	LDA	C9-C10-C11-C12
3	B	1305	LDA	C5-C6-C7-C8
3	B	1316	LDA	C11-C10-C9-C8
3	C	1294	LDA	C11-C10-C9-C8
3	D	1302	LDA	C4-C5-C6-C7
3	B	1312	LDA	C1-C2-C3-C4
3	D	1310	LDA	C3-C4-C5-C6
3	C	1292	LDA	C3-C4-C5-C6
3	B	1313	LDA	C2-C3-C4-C5
3	B	1305	LDA	C11-C10-C9-C8
3	C	1314	LDA	C5-C6-C7-C8
3	A	1292	LDA	C3-C4-C5-C6
3	C	1304	LDA	C7-C8-C9-C10
3	C	1303	LDA	C5-C6-C7-C8
3	D	1300	LDA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	A	1312	LDA	C5-C6-C7-C8
3	C	1307	LDA	C7-C8-C9-C10
3	D	1313	LDA	C3-C4-C5-C6
3	B	1302	LDA	C9-C10-C11-C12
3	C	1322	LDA	C9-C10-C11-C12
3	A	1301	LDA	C4-C5-C6-C7
3	C	1303	LDA	C11-C10-C9-C8
3	B	1323	LDA	C7-C8-C9-C10
3	C	1306	LDA	C9-C10-C11-C12
3	A	1325	LDA	C7-C8-C9-C10
3	B	1311	LDA	C9-C10-C11-C12
3	C	1307	LDA	C9-C10-C11-C12
3	A	1294	LDA	C6-C7-C8-C9
3	D	1312	LDA	C9-C10-C11-C12
3	B	1301	LDA	C11-C10-C9-C8
3	C	1300	LDA	C6-C7-C8-C9
3	C	1301	LDA	C4-C5-C6-C7
3	C	1289	LDA	C3-C4-C5-C6
3	B	1330	LDA	C7-C8-C9-C10
3	B	1324	LDA	C2-C3-C4-C5
3	B	1307	LDA	C5-C6-C7-C8
3	C	1328	LDA	C5-C6-C7-C8
3	D	1293	LDA	C3-C4-C5-C6
3	A	1293	LDA	C5-C6-C7-C8
3	C	1294	LDA	C6-C7-C8-C9
3	B	1318	LDA	C4-C5-C6-C7
3	D	1308	LDA	C5-C6-C7-C8
3	D	1295	LDA	C9-C10-C11-C12
3	A	413	LDA	C4-C5-C6-C7
3	B	1300	LDA	C4-C5-C6-C7
3	C	1281	LDA	C7-C8-C9-C10
3	B	1290	LDA	C3-C4-C5-C6
3	A	1310	LDA	C3-C4-C5-C6
3	A	1310	LDA	C5-C6-C7-C8
3	B	1316	LDA	C3-C4-C5-C6
3	B	482	LDA	C2-C3-C4-C5
3	C	1290	LDA	C3-C4-C5-C6
3	B	1302	LDA	C4-C5-C6-C7
3	B	1308	LDA	C7-C8-C9-C10
3	C	1297	LDA	C3-C4-C5-C6
3	D	1281	LDA	C9-C10-C11-C12
3	D	1300	LDA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	A	1320	LDA	C4-C5-C6-C7
3	C	1314	LDA	C7-C8-C9-C10
3	D	1298	LDA	C9-C10-C11-C12
3	D	1290	LDA	C3-C4-C5-C6
3	A	1321	LDA	C4-C5-C6-C7
3	B	1294	LDA	C5-C6-C7-C8
3	B	1298	LDA	C9-C10-C11-C12
3	A	1325	LDA	C4-C5-C6-C7
3	A	1315	LDA	C5-C6-C7-C8
3	B	1319	LDA	C3-C4-C5-C6
3	D	1298	LDA	C3-C4-C5-C6
3	C	1299	LDA	C4-C5-C6-C7
3	C	1294	LDA	C4-C5-C6-C7
3	D	1301	LDA	C4-C5-C6-C7
3	D	1295	LDA	C11-C10-C9-C8
3	D	1305	LDA	C11-C10-C9-C8
3	D	1293	LDA	C7-C8-C9-C10
3	C	1311	LDA	C4-C5-C6-C7
3	C	1290	LDA	C9-C10-C11-C12
3	A	1299	LDA	C4-C5-C6-C7
3	B	1298	LDA	C3-C4-C5-C6
3	C	1309	LDA	C6-C7-C8-C9
3	D	1306	LDA	C7-C8-C9-C10
3	B	1323	LDA	C4-C5-C6-C7
3	B	413	LDA	C4-C5-C6-C7
3	D	1294	LDA	C5-C6-C7-C8
3	B	1317	LDA	C6-C7-C8-C9
3	B	1308	LDA	N1-C1-C2-C3
3	C	1281	LDA	C11-C10-C9-C8
3	C	1328	LDA	C6-C7-C8-C9
3	C	1314	LDA	C9-C10-C11-C12
3	B	482	LDA	C5-C6-C7-C8
3	C	1297	LDA	C9-C10-C11-C12
3	B	1314	LDA	C2-C3-C4-C5
3	B	1327	LDA	C3-C4-C5-C6
3	C	413	LDA	C4-C5-C6-C7
3	C	1298	LDA	C7-C8-C9-C10
3	A	1326	LDA	C7-C8-C9-C10
3	A	1307	LDA	C2-C1-N1-CM2
3	A	1308	LDA	C2-C1-N1-CM2
3	B	1319	LDA	C2-C1-N1-CM1
3	B	1330	LDA	C2-C1-N1-CM1

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Mol	Chain	Res	Type	Atoms
3	D	1299	LDA	C2-C1-N1-CM1
3	D	1304	LDA	C2-C1-N1-CM2
3	C	1293	LDA	C5-C6-C7-C8
3	A	1308	LDA	C7-C8-C9-C10
3	A	1327	LDA	C9-C10-C11-C12
3	C	1296	LDA	C6-C7-C8-C9
3	B	1319	LDA	C2-C3-C4-C5
3	A	1289	LDA	C3-C4-C5-C6
3	B	1312	LDA	C9-C10-C11-C12
3	C	1313	LDA	C5-C6-C7-C8
3	A	1306	LDA	C7-C8-C9-C10
3	B	1295	LDA	C4-C5-C6-C7
3	B	1306	LDA	C3-C4-C5-C6
3	D	1291	LDA	C3-C4-C5-C6
3	D	1309	LDA	C5-C6-C7-C8
3	C	1310	LDA	C2-C3-C4-C5
3	C	1321	LDA	C9-C10-C11-C12
3	A	1292	LDA	C7-C8-C9-C10
3	D	1282	LDA	C7-C8-C9-C10
3	B	1313	LDA	C7-C8-C9-C10
3	A	1294	LDA	C9-C10-C11-C12
3	C	1305	LDA	C9-C10-C11-C12
3	A	1320	LDA	C2-C3-C4-C5
3	C	1327	LDA	C7-C8-C9-C10
3	A	1293	LDA	C2-C1-N1-O1
3	A	1301	LDA	C2-C1-N1-O1
3	A	1318	LDA	C2-C1-N1-O1
3	B	1294	LDA	C2-C1-N1-O1
3	B	1302	LDA	C2-C1-N1-O1
3	B	1316	LDA	C2-C1-N1-O1
3	B	1320	LDA	C2-C1-N1-O1
3	B	1323	LDA	C2-C1-N1-O1
3	B	1330	LDA	C2-C1-N1-O1
3	C	1293	LDA	C2-C1-N1-O1
3	C	1301	LDA	C2-C1-N1-O1
3	C	1317	LDA	C2-C1-N1-O1
3	C	1318	LDA	C2-C1-N1-O1
3	C	1323	LDA	C2-C1-N1-O1
3	D	1294	LDA	C2-C1-N1-O1
3	D	1306	LDA	C2-C1-N1-O1
3	D	1309	LDA	C2-C1-N1-O1
3	A	1296	LDA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	D	1297	LDA	C6-C7-C8-C9
3	B	1295	LDA	C9-C10-C11-C12
3	B	1301	LDA	C9-C10-C11-C12
3	A	1312	LDA	C7-C8-C9-C10
3	C	1292	LDA	C7-C8-C9-C10
3	B	1309	LDA	C1-C2-C3-C4
3	C	1323	LDA	C3-C4-C5-C6
3	B	1293	LDA	C7-C8-C9-C10
3	C	1308	LDA	C7-C8-C9-C10
3	C	1326	LDA	C11-C10-C9-C8
3	C	1317	LDA	C7-C8-C9-C10
3	D	1295	LDA	C6-C7-C8-C9
3	C	1325	LDA	C9-C10-C11-C12

There are no ring outliers.

117 monomers are involved in 296 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1324	LDA	1	0
3	D	1298	LDA	2	0
3	D	1306	LDA	3	0
3	C	1302	LDA	1	0
3	A	1292	LDA	4	0
3	A	1318	LDA	9	0
3	C	1318	LDA	4	0
3	B	1323	LDA	1	0
3	C	1321	LDA	3	0
3	B	482	LDA	1	0
3	C	1304	LDA	1	0
3	C	1312	LDA	1	0
3	C	1319	LDA	4	0
3	C	1300	LDA	3	0
3	A	1297	LDA	2	0
3	A	1304	LDA	4	0
3	D	1307	LDA	10	0
3	D	1308	LDA	5	0
3	C	1313	LDA	4	0
3	B	1311	LDA	3	0
3	C	1305	LDA	1	0
3	C	1281	LDA	4	0
3	D	1295	LDA	3	0
3	A	1303	LDA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1323	LDA	7	0
3	B	1330	LDA	6	0
3	A	1316	LDA	2	0
3	B	1327	LDA	1	0
3	C	1310	LDA	1	0
3	D	1311	LDA	2	0
3	C	1325	LDA	1	0
3	C	1326	LDA	2	0
3	A	1300	LDA	8	0
3	A	1307	LDA	2	0
3	A	1308	LDA	5	0
3	A	1309	LDA	6	0
3	B	1329	LDA	6	0
3	A	1302	LDA	1	0
3	A	1315	LDA	9	0
3	D	1293	LDA	4	0
3	B	1299	LDA	5	0
3	C	1328	LDA	2	0
3	D	1312	LDA	1	0
3	D	1313	LDA	3	0
3	B	1301	LDA	8	0
3	A	1298	LDA	4	0
3	C	1298	LDA	5	0
3	B	1324	LDA	1	0
3	A	413	LDA	9	0
3	A	1323	LDA	1	0
3	A	1322	LDA	5	0
3	B	1306	LDA	3	0
3	B	1304	LDA	5	0
3	A	1306	LDA	2	0
3	B	1298	LDA	1	0
3	A	1324	LDA	3	0
3	A	1321	LDA	1	0
3	C	1309	LDA	2	0
3	D	1292	LDA	6	0
3	D	1299	LDA	6	0
3	C	1307	LDA	6	0
3	A	1320	LDA	6	0
3	D	1282	LDA	2	0
3	B	1313	LDA	5	0
3	A	1326	LDA	2	0
3	B	1300	LDA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1311	LDA	1	0
3	B	1307	LDA	4	0
3	B	1310	LDA	4	0
3	A	1291	LDA	7	0
3	B	1294	LDA	6	0
3	C	1291	LDA	11	0
3	C	1299	LDA	2	0
3	C	1292	LDA	4	0
3	B	1293	LDA	4	0
3	C	1327	LDA	3	0
3	B	1328	LDA	5	0
3	A	1310	LDA	6	0
3	C	1290	LDA	6	0
3	A	1299	LDA	1	0
3	B	1292	LDA	12	0
3	C	1308	LDA	7	0
3	A	1301	LDA	1	0
3	C	1320	LDA	2	0
3	C	413	LDA	3	0
3	B	1312	LDA	2	0
3	C	1294	LDA	4	0
3	B	1319	LDA	4	0
3	A	1325	LDA	4	0
3	C	1297	LDA	1	0
3	D	1304	LDA	1	0
3	A	1293	LDA	1	0
3	B	413	LDA	2	0
3	C	1315	LDA	4	0
3	B	1291	LDA	3	0
3	B	1295	LDA	1	0
3	B	1320	LDA	1	0
4	B	1289	TAM	1	0
3	D	1305	LDA	2	0
3	D	1281	LDA	1	0
3	A	1290	LDA	4	0
3	B	1309	LDA	1	0
3	B	1314	LDA	1	0
3	D	1310	LDA	1	0
3	C	1314	LDA	2	0
3	B	1315	LDA	2	0
3	D	1309	LDA	1	0
3	A	1319	LDA	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1301	LDA	10	0
3	A	1313	LDA	10	0
3	C	1303	LDA	2	0
3	A	1327	LDA	2	0
3	D	1291	LDA	6	0
3	C	1316	LDA	1	0
3	B	1326	LDA	8	0
3	B	1322	LDA	4	0
3	A	1294	LDA	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.