



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 01:19 AM EDT

PDB ID : 5NXR
Title : Trimeric structure of Omp-Pst1, the major porin from *Providencia stuartii*
Authors : Colletier, J.P.; Nasrallah, C.
Deposited on : 2017-05-10
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

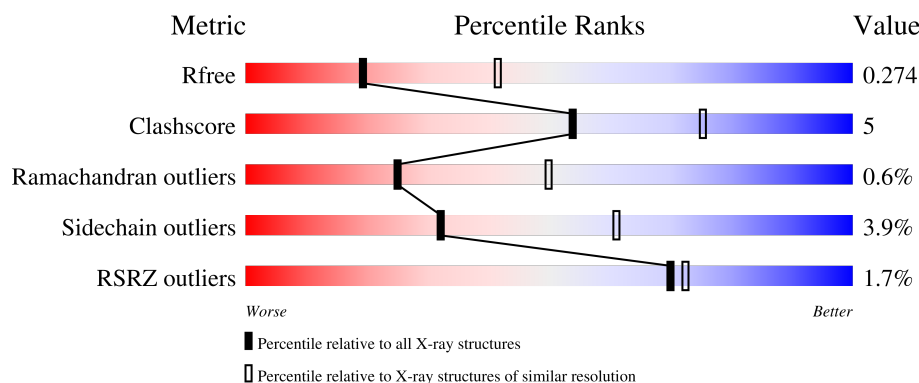
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	352	 2% 87% 11%
1	B	352	 % 85% 14%
1	C	352	 % 87% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LDA	A	401	-	-	-	X
2	LDA	A	405	-	-	-	X
2	LDA	A	406	-	-	-	X
2	LDA	A	407	-	-	-	X
2	LDA	A	408	-	-	-	X
2	LDA	A	411	-	-	-	X
2	LDA	A	412	-	-	-	X
2	LDA	B	401	-	-	-	X
2	LDA	B	407[A]	-	-	-	X
2	LDA	B	407[B]	-	-	-	X
2	LDA	B	410[A]	-	-	-	X
2	LDA	B	410[B]	-	-	-	X
2	LDA	B	411[A]	-	-	-	X
2	LDA	B	411[B]	-	-	-	X
2	LDA	B	417	-	-	-	X
2	LDA	C	409	-	-	-	X
2	LDA	C	410	-	-	-	X
2	LDA	C	421	-	-	-	X
2	LDA	C	424	-	-	-	X
2	LDA	C	428	-	-	-	X
2	LDA	C	431	-	-	-	X
2	LDA	C	432	-	-	-	X
2	LDA	C	433[A]	-	-	-	X
2	LDA	C	433[B]	-	-	-	X
2	LDA	C	434[A]	-	-	-	X
2	LDA	C	434[B]	-	-	-	X
2	LDA	C	435	-	-	-	X
2	LDA	C	436	-	-	-	X
2	LDA	C	438	-	-	-	X
2	LDA	C	440	-	-	-	X
2	LDA	C	442	-	-	-	X

2 Entry composition [i](#)

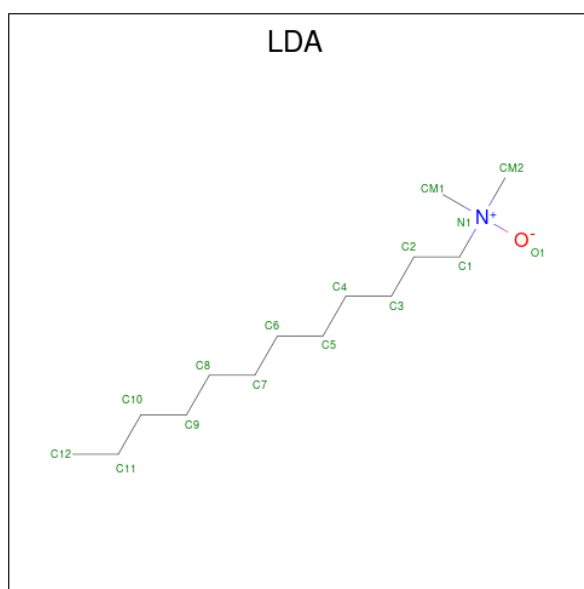
There are 5 unique types of molecules in this entry. The entry contains 10312 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Porin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	2	0
			2781	1744	472	560	5			
1	C	352	Total	C	N	O	S	0	3	0
			2782	1740	473	564	5			
1	B	352	Total	C	N	O	S	0	4	0
			2793	1749	475	564	5			

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



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	10	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			13	11	1	1		
2	A	1	Total	C	N	O	0	0
			12	10	1	1		
2	A	1	Total	C	N	O	0	0
			10	8	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			8	6	1	1		
2	A	1	Total	C	N	O	0	0
			11	9	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			10	8	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			13	11	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			11	9	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			10	8	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			9	7	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			13	11	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			15	13	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C			0	1
			22	22				
2	C	1	Total	C			0	1
			20	20				
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C			0	0
			12	12				
2	C	1	Total	C	N	O	0	0
			9	7	1	1		
2	C	1	Total	C	N	O	0	0
			11	9	1	1		
2	C	1	Total	C	N	O	0	0
			11	9	1	1		
2	C	1	Total	C			0	0
			9	9				
2	C	1	Total	C			0	0
			9	9				
2	C	1	Total	C			0	0
			9	9				
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	1
			32	28	2	2		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	1
			32	28	2	2		
2	B	1	Total	C	N	O	0	0
			13	11	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	1
			32	28	2	2		
2	B	1	Total	C	N	O	0	1
			32	28	2	2		

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

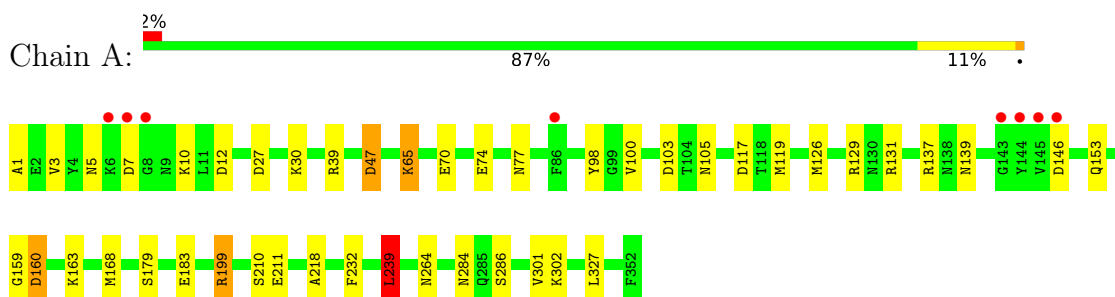
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	276	Total	O	0	0
			276	276		
5	C	305	Total	O	0	0
			305	305		
5	B	253	Total	O	0	0
			253	253		

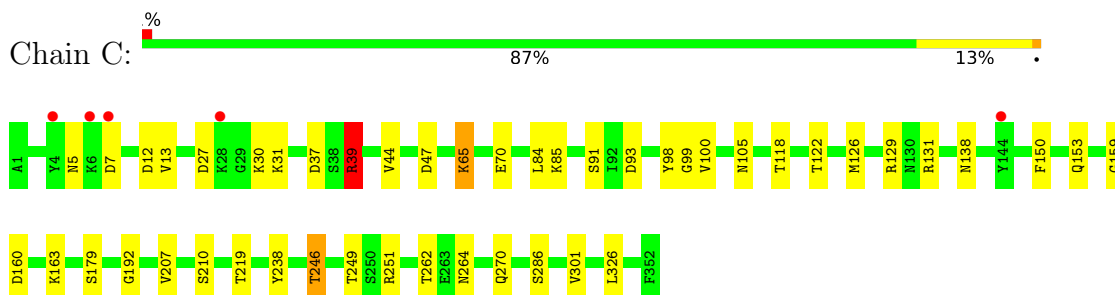
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

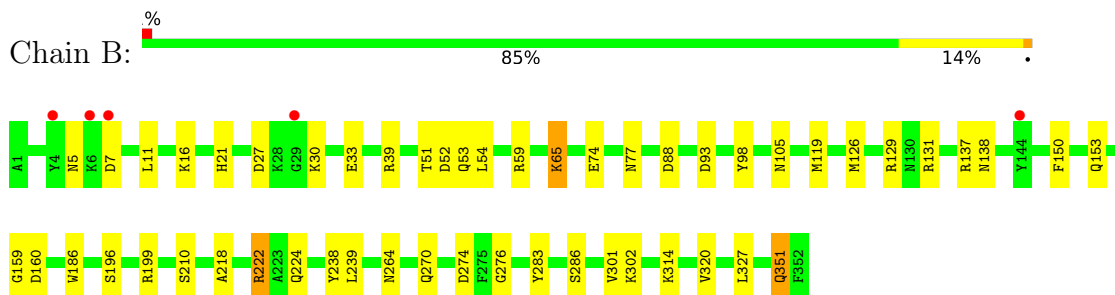
• Molecule 1: Porin 1



• Molecule 1: Porin 1



• Molecule 1: Porin 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.84Å 129.00Å 159.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-2.70) 95.3 (19.99-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.237 , 0.285 0.228 , 0.274	Depositor DCC
R_{free} test set	2960 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10312	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.66	0/2840	0.91	7/3835 (0.2%)
1	B	0.69	0/2850	0.86	5/3845 (0.1%)
1	C	0.69	0/2839	0.84	3/3833 (0.1%)
All	All	0.68	0/8529	0.87	15/11513 (0.1%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	ARG	NE-CZ-NH2	17.71	129.15	120.30
1	A	137	ARG	NE-CZ-NH1	-11.24	114.68	120.30
1	B	239	LEU	CB-CG-CD2	-7.70	97.91	111.00
1	C	12	ASP	CB-CG-OD2	6.93	124.54	118.30
1	A	146	ASP	N-CA-C	6.75	129.21	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	2781	0	2605	25	0
1	B	2793	0	2623	26	0
1	C	2782	0	2602	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	178	0	325	7	0
2	B	333	0	642	10	0
2	C	609	0	1137	17	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	276	0	0	3	0
5	B	253	0	0	2	0
5	C	305	0	0	6	0
All	All	10312	0	9934	102	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 5.

The worst 5 of 102 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:122:THR:O	1:C:251:ARG:NH1	2.16	0.78
1:C:100:VAL:H	1:C:153:GLN:HE22	1.33	0.77
1:C:37:ASP:O	1:C:39:ARG:NH1	2.21	0.73
1:A:302:LYS:HB3	1:A:327:LEU:HD12	1.76	0.67
1:C:100:VAL:H	1:C:153:GLN:NE2	1.92	0.67

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	352/352 (100%)	324 (92%)	26 (7%)	2 (1%)	25	50
1	B	354/352 (101%)	326 (92%)	26 (7%)	2 (1%)	25	50
1	C	353/352 (100%)	324 (92%)	27 (8%)	2 (1%)	25	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1059/1056 (100%)	974 (92%)	79 (8%)	6 (1%)	25 50

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	7	ASP
1	A	7	ASP
1	A	160	ASP
1	C	160	ASP
1	B	7	ASP

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	286/284 (101%)	275 (96%)	11 (4%)	33 62
1	B	288/284 (101%)	275 (96%)	13 (4%)	27 55
1	C	287/284 (101%)	277 (96%)	10 (4%)	36 65
All	All	861/852 (101%)	827 (96%)	34 (4%)	32 61

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	131	ARG
1	B	210	SER
1	B	314[B]	LYS
1	C	39	ARG
1	C	5	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	21	HIS
1	B	75	ASN

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Mol	Chain	Res	Type
1	B	285	GLN
1	B	235	ASN
1	B	245	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 80 ligands modelled in this entry, 2 are monoatomic - leaving 78 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	$\# Z > 2$
2	LDA	C	407	-	12,15,15	0.73	0	14,17,17	0.65	0
2	LDA	C	403	-	12,15,15	0.77	1 (8%)	14,17,17	0.60	0
2	LDA	A	403	-	12,15,15	0.90	1 (8%)	14,17,17	0.64	0
2	LDA	A	412	-	4,7,15	1.05	1 (25%)	6,9,17	5.09	3 (50%)
2	LDA	C	433[B]	-	10,10,15	0.43	0	9,9,17	0.48	0
2	LDA	A	407	-	9,12,15	0.83	0	11,14,17	3.63	3 (27%)
2	LDA	B	404	-	12,15,15	1.13	1 (8%)	14,17,17	0.93	0
2	LDA	A	405	-	12,15,15	0.67	0	14,17,17	1.01	1 (7%)
2	LDA	B	416	-	12,15,15	0.87	1 (8%)	14,17,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LDA	C	431	-	12,15,15	0.68	0	14,17,17	0.82	1 (7%)
2	LDA	A	413	-	7,10,15	0.72	0	9,12,17	3.62	3 (33%)
2	LDA	A	401	-	12,15,15	0.85	1 (8%)	14,17,17	0.67	0
2	LDA	C	438	-	7,10,15	0.96	0	9,12,17	3.68	3 (33%)
2	LDA	C	425	-	12,15,15	0.87	1 (8%)	14,17,17	0.75	1 (7%)
2	LDA	C	404	-	12,15,15	1.00	1 (8%)	14,17,17	0.74	1 (7%)
2	LDA	C	416	-	6,9,15	0.98	0	8,11,17	0.95	0
2	LDA	A	402	-	12,15,15	0.85	1 (8%)	14,17,17	0.92	0
2	LDA	C	406	-	12,15,15	0.91	1 (8%)	14,17,17	0.63	0
2	LDA	C	412	-	12,15,15	0.94	1 (8%)	14,17,17	0.84	1 (7%)
2	LDA	B	413	-	12,15,15	0.89	1 (8%)	14,17,17	0.70	0
2	LDA	B	401	-	12,15,15	0.75	1 (8%)	14,17,17	0.63	0
2	LDA	C	415	-	12,15,15	0.78	1 (8%)	14,17,17	0.65	0
2	LDA	B	405	-	12,15,15	0.85	1 (8%)	14,17,17	0.72	0
2	LDA	C	405	-	9,12,15	1.13	1 (11%)	11,14,17	0.94	1 (9%)
2	LDA	C	417	-	12,15,15	0.81	0	14,17,17	0.94	1 (7%)
2	LDA	C	436	-	11,11,15	0.47	0	10,10,17	0.44	0
2	LDA	C	420	-	12,15,15	1.27	1 (8%)	14,17,17	0.73	0
2	LDA	C	413	-	12,15,15	0.81	1 (8%)	14,17,17	0.73	1 (7%)
2	LDA	C	424	-	5,8,15	0.94	0	7,10,17	0.84	0
2	LDA	A	409	-	6,9,15	0.94	0	8,11,17	0.45	0
2	LDA	B	411[B]	-	12,15,15	0.71	0	14,17,17	0.34	0
2	LDA	B	415	-	12,15,15	0.84	1 (8%)	14,17,17	0.53	0
2	LDA	A	408	-	8,11,15	0.86	1 (12%)	10,13,17	0.79	0
2	LDA	C	437	-	5,8,15	1.05	1 (20%)	7,10,17	0.62	0
2	LDA	C	434[B]	-	9,9,15	0.41	0	8,8,17	0.47	0
2	LDA	C	428	-	12,15,15	0.71	0	14,17,17	3.23	3 (21%)
2	LDA	B	409	-	12,15,15	0.84	0	14,17,17	0.72	1 (7%)
2	LDA	B	406	-	12,15,15	0.85	1 (8%)	14,17,17	3.18	3 (21%)
2	LDA	B	417	-	12,15,15	0.80	1 (8%)	14,17,17	3.40	3 (21%)
2	LDA	C	421	-	12,15,15	0.85	1 (8%)	14,17,17	0.74	0
2	LDA	B	410[A]	-	12,15,15	0.66	0	14,17,17	0.71	0
2	LDA	B	407[A]	-	12,15,15	0.68	0	14,17,17	3.29	3 (21%)
2	LDA	C	439	-	7,10,15	0.68	0	9,12,17	3.83	3 (33%)
2	LDA	C	418	-	12,15,15	1.18	1 (8%)	14,17,17	0.57	0
2	LDA	B	402[B]	-	12,15,15	0.68	0	14,17,17	3.22	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LDA	C	441	-	8,8,15	0.47	0	7,7,17	0.39	0
2	LDA	C	430	-	12,15,15	0.89	1 (8%)	14,17,17	0.61	0
2	LDA	C	410	-	7,10,15	0.96	1 (14%)	9,12,17	0.61	0
2	LDA	C	409	-	12,15,15	0.82	1 (8%)	14,17,17	0.61	0
2	LDA	C	423	-	12,15,15	0.97	1 (8%)	14,17,17	0.64	0
2	LDA	C	426	-	12,15,15	0.85	1 (8%)	14,17,17	0.81	0
2	LDA	C	433[A]	-	10,10,15	0.42	0	9,9,17	0.49	0
2	LDA	C	411	-	12,15,15	0.91	1 (8%)	14,17,17	0.64	0
2	LDA	C	401	-	12,15,15	0.91	1 (8%)	14,17,17	0.66	0
2	LDA	B	411[A]	-	12,15,15	0.78	1 (8%)	14,17,17	0.46	0
2	LDA	C	440	-	8,8,15	0.53	0	7,7,17	0.34	0
2	LDA	A	411	-	12,15,15	0.62	0	14,17,17	1.12	1 (7%)
2	LDA	C	402	-	6,9,15	1.11	1 (16%)	8,11,17	0.88	1 (12%)
2	LDA	B	408	-	9,12,15	0.73	0	11,14,17	0.57	0
2	LDA	B	402[A]	-	12,15,15	0.75	1 (8%)	14,17,17	0.41	0
2	LDA	A	410	-	12,15,15	0.82	1 (8%)	14,17,17	0.81	1 (7%)
2	LDA	B	403	-	12,15,15	0.95	1 (8%)	14,17,17	0.46	0
2	LDA	C	432	-	12,15,15	0.71	0	14,17,17	0.60	0
2	LDA	C	419	-	12,15,15	0.67	0	14,17,17	0.87	1 (7%)
2	LDA	C	435	-	12,15,15	0.77	0	14,17,17	3.12	3 (21%)
2	LDA	C	414	-	12,15,15	0.80	1 (8%)	14,17,17	0.63	0
2	LDA	C	427	-	9,12,15	0.93	1 (11%)	11,14,17	0.72	0
2	LDA	B	412	-	12,15,15	0.73	0	14,17,17	1.11	1 (7%)
2	LDA	C	434[A]	-	9,9,15	0.43	0	8,8,17	0.45	0
2	LDA	C	442	-	8,8,15	0.59	0	7,7,17	0.26	0
2	LDA	B	410[B]	-	12,15,15	0.56	0	14,17,17	0.49	0
2	LDA	B	407[B]	-	12,15,15	0.66	0	14,17,17	3.17	3 (21%)
2	LDA	B	414	-	12,15,15	0.51	0	14,17,17	3.65	3 (21%)
2	LDA	C	429	-	11,13,15	0.80	1 (9%)	10,14,17	0.46	0
2	LDA	A	406	-	12,15,15	0.73	0	14,17,17	3.28	3 (21%)
2	LDA	C	408	-	12,15,15	0.69	0	14,17,17	3.08	3 (21%)
2	LDA	A	404	-	8,11,15	0.98	1 (12%)	10,13,17	0.73	0
2	LDA	C	422	-	12,15,15	0.72	0	14,17,17	3.21	3 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LDA	C	407	-	-	11/13/13/13	-
2	LDA	C	403	-	-	2/13/13/13	-
2	LDA	A	403	-	-	12/13/13/13	-
2	LDA	A	412	-	-	4/5/5/13	-
2	LDA	C	433[B]	-	-	8/8/8/13	-
2	LDA	A	407	-	-	7/10/10/13	-
2	LDA	B	404	-	-	9/13/13/13	-
2	LDA	A	405	-	-	12/13/13/13	-
2	LDA	B	416	-	-	7/13/13/13	-
2	LDA	C	431	-	-	11/13/13/13	-
2	LDA	A	413	-	-	7/8/8/13	-
2	LDA	A	401	-	-	6/13/13/13	-
2	LDA	C	438	-	-	6/8/8/13	-
2	LDA	C	425	-	-	9/13/13/13	-
2	LDA	C	404	-	-	12/13/13/13	-
2	LDA	C	416	-	-	0/7/7/13	-
2	LDA	A	402	-	-	8/13/13/13	-
2	LDA	C	406	-	-	5/13/13/13	-
2	LDA	C	412	-	-	5/13/13/13	-
2	LDA	B	413	-	-	2/13/13/13	-
2	LDA	B	401	-	-	11/13/13/13	-
2	LDA	C	415	-	-	1/13/13/13	-
2	LDA	B	405	-	-	6/13/13/13	-
2	LDA	C	405	-	-	4/10/10/13	-
2	LDA	C	417	-	-	9/13/13/13	-
2	LDA	C	436	-	-	8/9/9/13	-
2	LDA	C	420	-	-	8/13/13/13	-
2	LDA	C	413	-	-	6/13/13/13	-
2	LDA	C	424	-	-	1/6/6/13	-
2	LDA	A	409	-	-	4/7/7/13	-
2	LDA	B	411[B]	-	-	4/13/13/13	-
2	LDA	B	415	-	-	11/13/13/13	-
2	LDA	A	408	-	-	8/9/9/13	-
2	LDA	C	437	-	-	3/6/6/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LDA	C	434[B]	-	-	5/7/7/13	-
2	LDA	C	428	-	-	9/13/13/13	-
2	LDA	B	409	-	-	9/13/13/13	-
2	LDA	B	406	-	-	3/13/13/13	-
2	LDA	B	417	-	-	9/13/13/13	-
2	LDA	C	421	-	-	8/13/13/13	-
2	LDA	B	410[A]	-	-	12/13/13/13	-
2	LDA	B	407[A]	-	-	6/13/13/13	-
2	LDA	C	439	-	-	6/8/8/13	-
2	LDA	C	418	-	-	3/13/13/13	-
2	LDA	B	402[B]	-	-	5/13/13/13	-
2	LDA	C	441	-	-	4/6/6/13	-
2	LDA	C	430	-	-	5/13/13/13	-
2	LDA	C	410	-	-	4/8/8/13	-
2	LDA	C	409	-	-	6/13/13/13	-
2	LDA	C	423	-	-	1/13/13/13	-
2	LDA	C	426	-	-	7/13/13/13	-
2	LDA	C	433[A]	-	-	6/8/8/13	-
2	LDA	C	411	-	-	3/13/13/13	-
2	LDA	C	401	-	-	8/13/13/13	-
2	LDA	B	411[A]	-	-	11/13/13/13	-
2	LDA	C	440	-	-	4/6/6/13	-
2	LDA	A	411	-	-	12/13/13/13	-
2	LDA	C	402	-	-	2/7/7/13	-
2	LDA	B	408	-	-	5/10/10/13	-
2	LDA	B	402[A]	-	-	11/13/13/13	-
2	LDA	A	410	-	-	10/13/13/13	-
2	LDA	B	403	-	-	5/13/13/13	-
2	LDA	C	432	-	-	9/13/13/13	-
2	LDA	C	419	-	-	6/13/13/13	-
2	LDA	C	435	-	-	8/13/13/13	-
2	LDA	C	414	-	-	11/13/13/13	-
2	LDA	C	427	-	-	5/10/10/13	-
2	LDA	B	412	-	-	9/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LDA	C	434[A]	-	-	2/7/7/13	-
2	LDA	C	442	-	-	3/6/6/13	-
2	LDA	B	410[B]	-	-	6/13/13/13	-
2	LDA	B	407[B]	-	-	8/13/13/13	-
2	LDA	B	414	-	-	8/13/13/13	-
2	LDA	C	429	-	-	7/9/9/13	-
2	LDA	A	406	-	-	9/13/13/13	-
2	LDA	C	408	-	-	9/13/13/13	-
2	LDA	A	404	-	-	5/9/9/13	-
2	LDA	C	422	-	-	3/13/13/13	-

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	420	LDA	O1-N1	3.93	1.51	1.42
2	B	404	LDA	O1-N1	3.44	1.50	1.42
2	C	418	LDA	O1-N1	3.29	1.49	1.42
2	C	405	LDA	O1-N1	3.01	1.49	1.42
2	C	401	LDA	O1-N1	2.86	1.48	1.42

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	414	LDA	O1-N1-C1	-11.82	80.27	109.27
2	A	412	LDA	O1-N1-C1	-10.65	83.15	109.27
2	B	407[A]	LDA	O1-N1-C1	-10.50	83.52	109.27
2	B	417	LDA	O1-N1-C1	-10.47	83.60	109.27
2	C	428	LDA	O1-N1-C1	-10.23	84.19	109.27

There are no chirality outliers.

5 of 514 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	LDA	C2-C1-N1-CM2
2	A	402	LDA	N1-C1-C2-C3
2	A	403	LDA	C2-C1-N1-O1
2	A	403	LDA	C2-C1-N1-CM2
2	A	403	LDA	N1-C1-C2-C3

There are no ring outliers.

35 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	403	LDA	1	0
2	A	412	LDA	2	0
2	B	404	LDA	1	0
2	B	416	LDA	1	0
2	A	413	LDA	2	0
2	C	425	LDA	1	0
2	C	416	LDA	2	0
2	C	406	LDA	1	0
2	C	412	LDA	2	0
2	B	413	LDA	1	0
2	C	415	LDA	1	0
2	B	405	LDA	3	0
2	C	405	LDA	2	0
2	C	417	LDA	2	0
2	C	420	LDA	2	0
2	C	413	LDA	2	0
2	A	409	LDA	2	0
2	A	408	LDA	1	0
2	B	417	LDA	1	0
2	B	402[B]	LDA	1	0
2	C	410	LDA	2	0
2	C	426	LDA	1	0
2	C	401	LDA	1	0
2	B	411[A]	LDA	1	0
2	B	402[A]	LDA	1	0
2	A	410	LDA	1	0
2	B	403	LDA	2	0
2	C	432	LDA	1	0
2	C	419	LDA	2	0
2	C	414	LDA	1	0
2	B	410[B]	LDA	1	0
2	B	414	LDA	1	0
2	C	429	LDA	1	0
2	A	406	LDA	1	0
2	C	408	LDA	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	352/352 (100%)	-0.23	8 (2%) 60 62	48, 69, 116, 145	0
1	B	352/352 (100%)	-0.34	5 (1%) 75 77	49, 67, 104, 156	0
1	C	352/352 (100%)	-0.28	5 (1%) 75 77	48, 65, 104, 150	0
All	All	1056/1056 (100%)	-0.28	18 (1%) 70 72	48, 67, 110, 156	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	ASP	4.9
1	A	86	PHE	4.1
1	C	7	ASP	3.6
1	A	6	LYS	3.5
1	C	28	LYS	3.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	LDA	C	409	16/16	0.20	0.68	99,155,225,234	0
2	LDA	C	431	16/16	0.24	0.47	136,186,208,210	0
2	LDA	C	434[A]	10/16	0.33	0.69	80,86,91,91	10
2	LDA	C	434[B]	10/16	0.33	0.69	71,85,90,91	10
2	LDA	C	435	16/16	0.33	0.77	165,185,192,194	0
2	LDA	C	442	9/16	0.35	0.44	102,112,124,126	0
2	LDA	C	436	12/16	0.36	0.54	151,173,191,194	0
2	LDA	C	432	16/16	0.36	0.44	156,188,201,204	0
2	LDA	C	424	9/16	0.40	0.72	130,167,186,191	0
2	LDA	C	438	11/16	0.41	0.57	119,159,166,168	0
2	LDA	B	407[A]	16/16	0.49	0.63	68,74,80,82	16
2	LDA	B	407[B]	16/16	0.49	0.63	64,82,87,87	16
2	LDA	A	407	13/16	0.50	0.64	114,167,188,189	0
2	LDA	B	412	16/16	0.50	0.34	101,123,164,165	0
2	LDA	C	421	16/16	0.53	0.42	116,130,152,154	0
2	LDA	A	409	10/16	0.53	0.40	141,166,185,186	0
2	LDA	C	410	11/16	0.53	0.43	105,168,202,203	0
2	LDA	C	440	9/16	0.53	0.46	108,122,132,136	0
2	LDA	B	417	16/16	0.55	0.42	73,149,205,206	0
2	LDA	C	433[B]	11/16	0.57	0.46	64,68,70,70	11
2	LDA	C	433[A]	11/16	0.57	0.46	76,82,83,83	11
2	LDA	A	411	16/16	0.60	0.57	89,126,196,201	0
2	LDA	A	401	16/16	0.60	0.45	63,113,187,194	0
2	LDA	C	420	16/16	0.62	0.36	74,80,120,124	0
2	LDA	B	410[B]	16/16	0.64	0.42	33,36,38,40	16
2	LDA	A	408	12/16	0.64	0.52	130,180,194,199	0
2	LDA	B	410[A]	16/16	0.64	0.42	62,70,76,77	16
2	LDA	A	405	16/16	0.66	0.44	77,130,155,162	0
2	LDA	C	406	16/16	0.66	0.34	69,99,149,156	0
2	LDA	C	412	16/16	0.67	0.30	82,97,158,161	0
2	LDA	A	406	16/16	0.67	0.47	87,114,134,138	0
2	LDA	C	408	16/16	0.67	0.34	62,121,187,191	0
2	LDA	A	404	12/16	0.69	0.34	109,112,143,145	0
2	LDA	C	430	16/16	0.71	0.36	97,106,121,124	0
2	LDA	C	419	16/16	0.71	0.38	92,140,151,154	0
2	LDA	C	423	16/16	0.72	0.31	75,89,165,175	0
2	LDA	C	428	16/16	0.72	0.61	128,186,194,196	0
2	LDA	C	441	9/16	0.73	0.38	116,136,145,147	0
2	LDA	A	413	11/16	0.73	0.39	133,164,193,194	0
2	LDA	C	437	9/16	0.74	0.26	92,107,140,151	0
2	LDA	B	402[A]	16/16	0.74	0.36	43,57,76,77	16
2	LDA	B	402[B]	16/16	0.74	0.36	47,52,85,89	16

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	LDA	C	411	16/16	0.75	0.22	64,97,137,142	0
2	LDA	A	412	8/16	0.76	0.51	116,148,170,179	0
2	LDA	B	401	16/16	0.76	0.40	73,104,142,143	0
2	LDA	C	418	16/16	0.77	0.26	47,66,100,102	0
2	LDA	C	427	13/16	0.78	0.25	73,98,143,145	0
2	LDA	C	413	16/16	0.78	0.26	60,71,125,129	0
2	LDA	C	439	11/16	0.78	0.27	106,113,119,121	0
2	LDA	C	429	15/16	0.78	0.33	56,64,172,173	0
2	LDA	C	422	16/16	0.78	0.21	70,90,168,179	0
2	LDA	B	415	16/16	0.79	0.39	73,101,138,142	0
2	LDA	C	402	10/16	0.79	0.23	67,100,133,134	0
2	LDA	B	411[B]	16/16	0.80	0.41	52,63,84,85	16
2	LDA	C	425	16/16	0.80	0.27	60,71,131,135	0
2	LDA	C	404	16/16	0.80	0.28	68,75,126,128	0
2	LDA	B	411[A]	16/16	0.80	0.41	55,66,80,81	16
2	LDA	C	405	13/16	0.81	0.27	70,80,116,117	0
2	LDA	A	403	16/16	0.81	0.36	80,96,123,124	0
2	LDA	C	407	16/16	0.81	0.26	50,63,120,124	0
2	LDA	C	415	16/16	0.81	0.23	75,89,135,138	0
2	LDA	B	416	16/16	0.81	0.23	68,100,145,146	0
2	LDA	C	426	16/16	0.81	0.26	61,84,173,173	0
2	LDA	C	416	10/16	0.82	0.26	42,52,82,88	0
2	LDA	C	414	16/16	0.84	0.22	69,82,118,118	0
2	LDA	B	414	16/16	0.85	0.30	72,89,132,132	0
2	LDA	B	409	16/16	0.85	0.23	49,93,124,128	0
2	LDA	B	406	16/16	0.85	0.20	51,93,151,160	0
2	LDA	B	408	13/16	0.85	0.19	54,64,95,105	0
2	LDA	C	417	16/16	0.86	0.26	53,67,103,104	0
2	LDA	B	405	16/16	0.87	0.24	62,84,168,171	0
2	LDA	A	410	16/16	0.88	0.18	65,89,148,148	0
2	LDA	B	403	16/16	0.88	0.20	61,78,87,88	0
2	LDA	B	404	16/16	0.88	0.21	50,62,75,75	0
2	LDA	C	401	16/16	0.89	0.17	55,76,127,128	0
2	LDA	C	403	16/16	0.90	0.19	47,63,85,87	0
2	LDA	A	402	16/16	0.90	0.23	54,63,104,107	0
4	CL	A	415	1/1	0.90	0.28	108,108,108,108	0
2	LDA	B	413	16/16	0.91	0.16	53,64,103,119	0
3	CA	A	414	1/1	0.96	0.30	80,80,80,80	0

6.5 Other polymers ⓘ

There are no such residues in this entry.