



# wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 03:58 PM EDT

PDB ID : 4LCZ  
Title : Crystal structure of a multilayer-packed major light-harvesting complex  
Authors : Wan, T.; Li, M.; Chang, W.R.  
Deposited on : 2013-06-24  
Resolution : 2.60 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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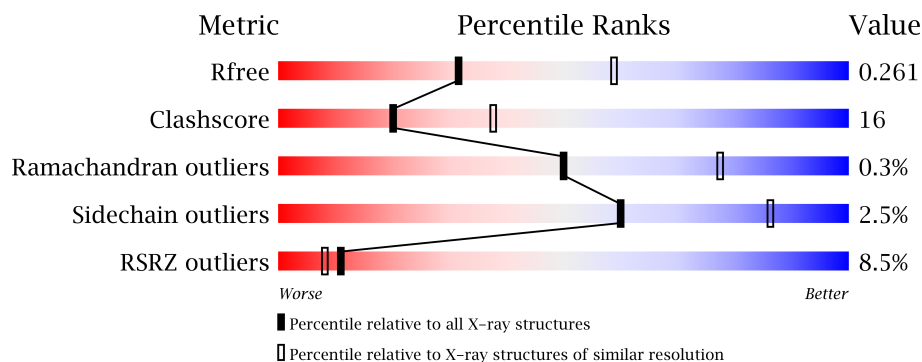
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23161  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23161

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	224	
1	B	224	
1	C	224	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NEX	A	303	-	X
3	NEX	B	303	-	X
4	LHG	A	304	-	X
4	LHG	B	304	-	X
5	CHL	A	309	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
6	CLA	A	306	-	X
6	CLA	A	307	-	X
6	CLA	B	307	-	X
6	CLA	B	316	-	X
6	CLA	C	307	-	X
7	CAC	A	319	X	-
7	CAC	B	319	X	-
7	CAC	C	319	X	-
9	NA	C	320	-	X
9	NA	C	323	-	X

## 2 Entry composition i

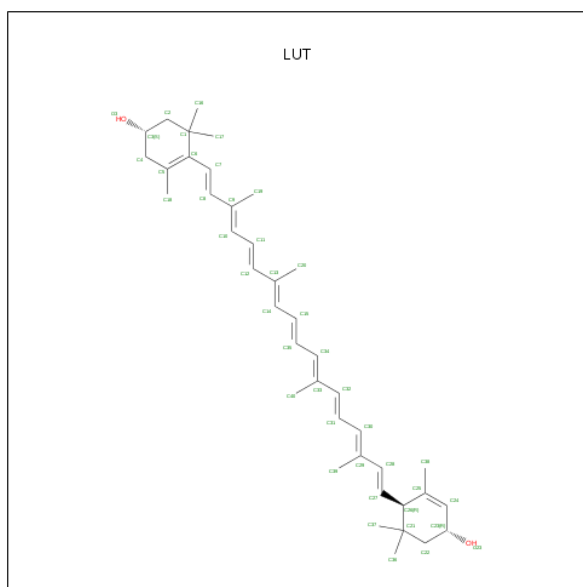
There are 10 unique types of molecules in this entry. The entry contains 8016 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Major chlorophyll a/b binding protein LHCb1.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1579	1023	257	292	7			
1	B	208	Total	C	N	O	S	0	0	0
			1579	1023	257	292	7			
1	C	208	Total	C	N	O	S	0	0	0
			1579	1023	257	292	7			

- Molecule 2 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



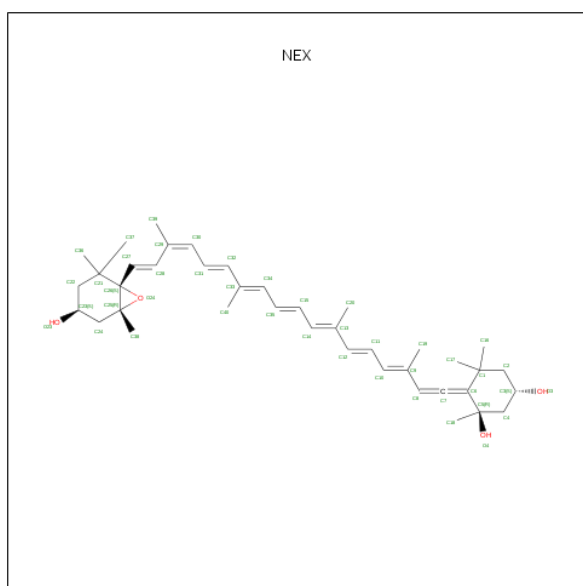
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			42	40	2		
2	A	1	Total	C	O	0	0
			42	40	2		
2	B	1	Total	C	O	0	0
			42	40	2		

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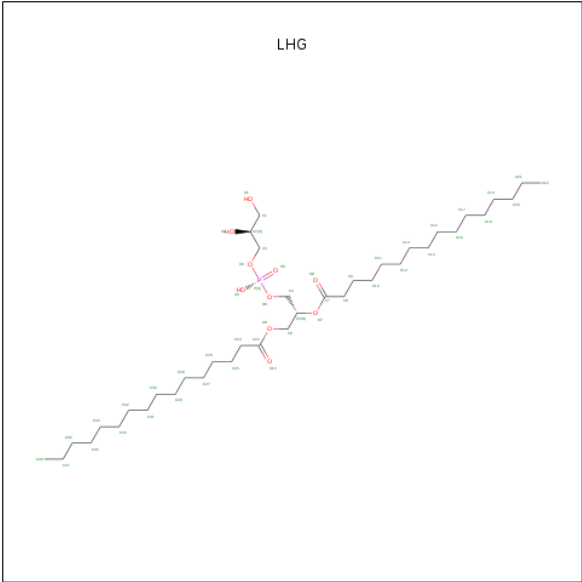
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			42	40	2		
2	C	1	Total	C	O	0	0
			42	40	2		
2	C	1	Total	C	O	0	0
			42	40	2		

- Molecule 3 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



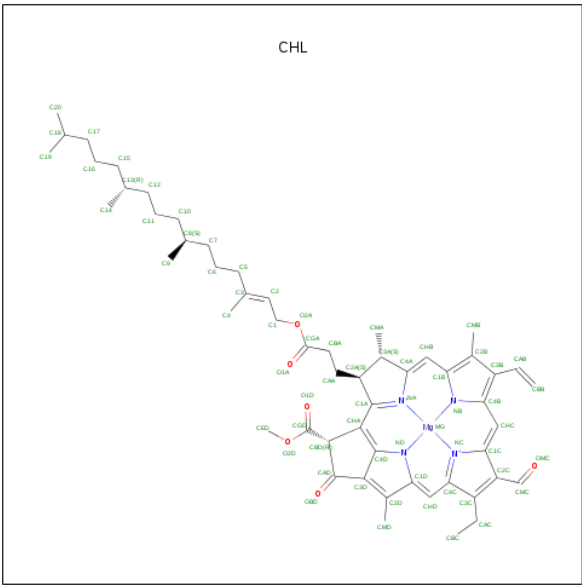
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			44	40	4		
3	B	1	Total	C	O	0	0
			44	40	4		
3	C	1	Total	C	O	0	0
			44	40	4		

- Molecule 4 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			49	38	10	1		
4	B	1	Total	C	O	P	0	0
			49	38	10	1		
4	C	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 5 is CHLOROPHYLL B (three-letter code: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).



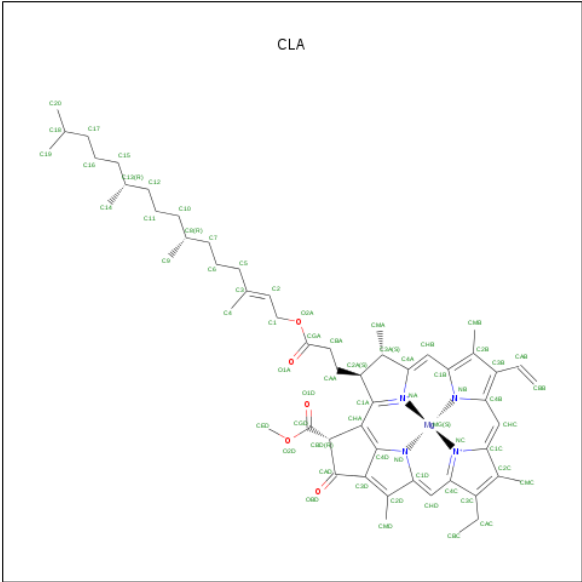
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
5	A	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
5	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			65	52	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

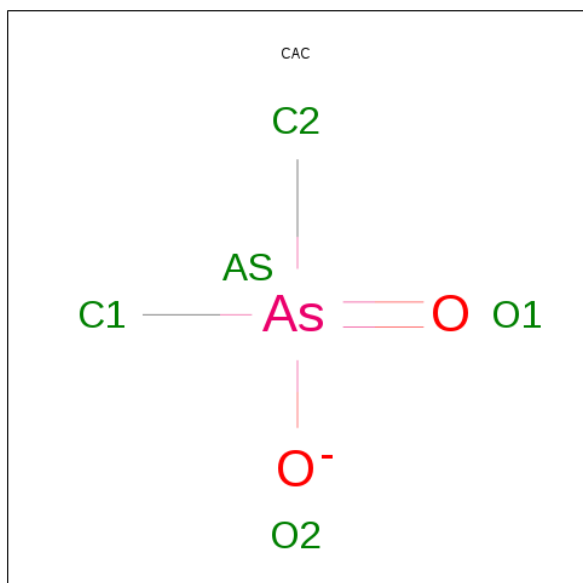
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			40	32	1	4	3		

- Molecule 7 is CACODYLATE ION (three-letter code: CAC) (formula:  $C_2H_6AsO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	As	C	O	0	0
			5	1	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	As	C	O	0	0
			5	1	2	2		
7	C	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Zn	0	0
			1	1		
8	A	3	Total	Zn	0	0
			3	3		
8	C	1	Total	Zn	0	0
			1	1		

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	2	Total	Na	0	0
			2	2		
9	C	3	Total	Na	0	0
			3	3		

- Molecule 10 is water.

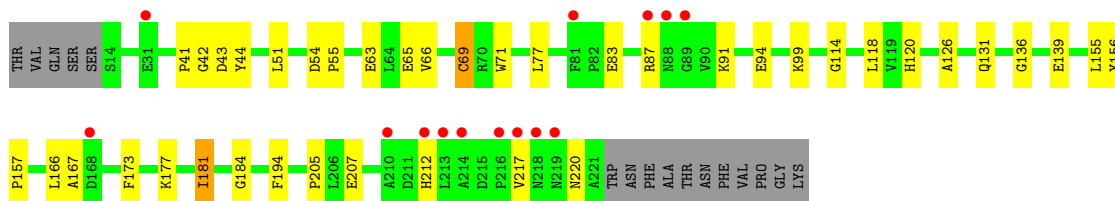
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	58	Total	O	0	0
			58	58		
10	B	46	Total	O	0	0
			46	46		
10	C	52	Total	O	0	0
			52	52		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

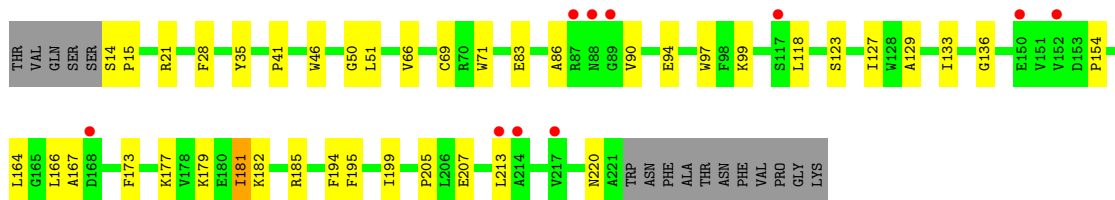
- Molecule 1: Major chlorophyll a/b binding protein LHCb1.3

Chain A: 



- Molecule 1: Major chlorophyll a/b binding protein LHCb1.3

Chain B: 



- Molecule 1: Major chlorophyll a/b binding protein LHCb1.3

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	199.19Å 115.10Å 109.60Å 90.00° 113.23° 90.00°	Depositor
Resolution (Å)	43.45 – 2.60 49.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.4 (43.45-2.60) 83.4 (49.97-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.06 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3.928)	Depositor
R, $R_{free}$	0.250 , 0.258 0.239 , 0.261	Depositor DCC
$R_{free}$ test set	2945 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 60677 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	8016	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, ZN, LUT, NA, CHL, CLA, NEX, CAC

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	0.51	1/1626 (0.1%)	0.60	0/2212
1	B	0.53	0/1626	0.60	0/2212
1	C	0.53	0/1626	0.64	0/2212
All	All	0.52	1/4878 (0.0%)	0.61	0/6636

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	CYS	CB-SG	-5.30	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1579	0	1520	33	0
1	B	1579	0	1521	31	0
1	C	1579	0	1521	20	0
2	A	84	0	112	6	0
2	B	84	0	112	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	84	0	112	7	0
3	A	44	0	56	3	0
3	B	44	0	56	3	0
3	C	44	0	56	3	0
4	A	49	0	74	9	0
4	B	49	0	74	5	0
4	C	49	0	74	5	0
5	A	363	0	350	23	0
5	B	363	0	350	22	0
5	C	363	0	350	21	0
6	A	493	0	522	43	0
6	B	493	0	524	43	0
6	C	492	0	521	47	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
8	A	3	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	B	2	0	0	0	0
9	C	3	0	0	0	0
10	A	58	0	0	1	0
10	B	46	0	0	2	0
10	C	52	0	0	2	0
All	All	8016	0	7905	250	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

The worst 5 of 250 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:C:304:LHG:C14	6:C:317:CLA:H93	1.72	1.19
6:C:306:CLA:H92	6:C:307:CLA:HMA1	1.20	1.14
4:A:304:LHG:H142	6:A:317:CLA:H93	1.22	1.12
4:A:304:LHG:C14	6:A:317:CLA:H93	1.83	1.08
6:B:306:CLA:H92	6:B:307:CLA:HMA1	1.32	1.08

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	206/224 (92%)	199 (97%)	6 (3%)	1 (0%)	38	67
1	B	206/224 (92%)	199 (97%)	7 (3%)	0	100	100
1	C	206/224 (92%)	198 (96%)	7 (3%)	1 (0%)	38	67
All	All	618/672 (92%)	596 (96%)	20 (3%)	2 (0%)	50	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	C	119	VAL

### 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	160/174 (92%)	157 (98%)	3 (2%)	69	91
1	B	160/174 (92%)	157 (98%)	3 (2%)	69	91
1	C	160/174 (92%)	154 (96%)	6 (4%)	44	74
All	All	480/522 (92%)	468 (98%)	12 (2%)	60	86

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	220	ASN
1	C	80	VAL
1	C	181	ILE
1	B	207	GLU

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Mol	Chain	Res	Type
1	C	96	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 67 ligands modelled in this entry, 10 are monoatomic - leaving 57 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	LUT	A	301	-	43,43,43	0.95	2 (4%)	60,60,60	1.57	11 (18%)
2	LUT	A	302	-	43,43,43	0.97	2 (4%)	60,60,60	1.56	12 (20%)
3	NEX	A	303	-	46,46,46	1.13	3 (6%)	70,70,70	2.93	22 (31%)
4	LHG	A	304	6	48,48,48	0.89	2 (4%)	54,54,54	1.04	4 (7%)
5	CHL	A	305	1	62,74,74	4.03	17 (27%)	52,114,114	1.79	11 (21%)
6	CLA	A	306	1	73,73,73	2.00	18 (24%)	96,113,113	2.34	27 (28%)
6	CLA	A	307	1	73,73,73	2.03	18 (24%)	96,113,113	2.21	34 (35%)
6	CLA	A	308	10	70,70,73	2.52	18 (25%)	92,109,113	2.43	24 (26%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	CHL	A	309	1	43,56,74	5.29	19 (44%)	29,92,114	2.27	9 (31%)
5	CHL	A	310	10	47,59,74	4.43	20 (42%)	32,96,114	2.11	9 (28%)
5	CHL	A	311	10	62,74,74	3.96	20 (32%)	52,114,114	1.68	8 (15%)
5	CHL	A	312	10	62,74,74	4.28	21 (33%)	52,114,114	1.64	9 (17%)
5	CHL	A	313	1	62,74,74	3.90	19 (30%)	52,114,114	1.60	8 (15%)
6	CLA	A	314	1	73,73,73	2.24	19 (26%)	96,113,113	2.12	28 (29%)
6	CLA	A	315	4	73,73,73	2.26	19 (26%)	96,113,113	2.20	31 (32%)
6	CLA	A	316	1	73,73,73	2.44	15 (20%)	96,113,113	2.23	29 (30%)
6	CLA	A	317	1	73,73,73	2.00	17 (23%)	96,113,113	2.21	31 (32%)
6	CLA	A	318	1	48,49,73	2.69	21 (43%)	65,84,113	2.27	23 (35%)
7	CAC	A	319	8	4,4,4	5.33	3 (75%)	6,6,6	18.37	5 (83%)
2	LUT	B	301	-	43,43,43	0.94	2 (4%)	60,60,60	1.70	16 (26%)
2	LUT	B	302	-	43,43,43	1.05	2 (4%)	60,60,60	1.77	15 (25%)
3	NEX	B	303	-	46,46,46	1.14	4 (8%)	70,70,70	2.93	23 (32%)
4	LHG	B	304	6	48,48,48	0.94	2 (4%)	54,54,54	1.10	3 (5%)
5	CHL	B	305	1	62,74,74	4.48	16 (25%)	52,114,114	1.64	9 (17%)
6	CLA	B	306	1	73,73,73	2.15	17 (23%)	96,113,113	2.34	35 (36%)
6	CLA	B	307	1	73,73,73	2.23	17 (23%)	96,113,113	2.33	30 (31%)
6	CLA	B	308	10	70,70,73	2.62	19 (27%)	92,109,113	2.42	23 (25%)
5	CHL	B	309	1	43,56,74	4.82	21 (48%)	29,92,114	2.35	9 (31%)
5	CHL	B	310	10	47,59,74	4.42	21 (44%)	32,96,114	2.47	10 (31%)
5	CHL	B	311	10	62,74,74	4.25	17 (27%)	52,114,114	1.73	9 (17%)
5	CHL	B	312	10	62,74,74	4.10	21 (33%)	52,114,114	1.59	8 (15%)
5	CHL	B	313	1	62,74,74	3.58	18 (29%)	52,114,114	1.73	11 (21%)
6	CLA	B	314	1	73,73,73	2.15	15 (20%)	96,113,113	2.29	27 (28%)
6	CLA	B	315	4	73,73,73	2.14	15 (20%)	96,113,113	2.25	31 (32%)
6	CLA	B	316	1	73,73,73	2.28	16 (21%)	96,113,113	2.17	30 (31%)
6	CLA	B	317	1	73,73,73	2.04	15 (20%)	96,113,113	2.27	28 (29%)
6	CLA	B	318	1	48,49,73	2.71	19 (39%)	65,84,113	2.33	20 (30%)
7	CAC	B	319	8	4,4,4	5.78	3 (75%)	6,6,6	24.59	5 (83%)
2	LUT	C	301	-	43,43,43	1.03	1 (2%)	60,60,60	1.96	18 (30%)
2	LUT	C	302	-	43,43,43	0.86	2 (4%)	60,60,60	1.92	13 (21%)
3	NEX	C	303	-	46,46,46	1.20	3 (6%)	70,70,70	3.06	22 (31%)
4	LHG	C	304	6	48,48,48	0.90	2 (4%)	54,54,54	1.01	3 (5%)
5	CHL	C	305	1	62,74,74	4.07	17 (27%)	52,114,114	1.76	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	CLA	C	306	1	73,73,73	2.34	17 (23%)	96,113,113	2.23	31 (32%)
6	CLA	C	307	1	73,73,73	2.02	17 (23%)	96,113,113	2.25	39 (40%)
6	CLA	C	308	10	70,70,73	2.23	18 (25%)	92,109,113	2.34	25 (27%)
5	CHL	C	309	1	43,56,74	5.09	20 (46%)	29,92,114	2.29	7 (24%)
5	CHL	C	310	10	47,59,74	4.38	23 (48%)	32,96,114	2.28	9 (28%)
5	CHL	C	311	10	62,74,74	4.20	18 (29%)	52,114,114	1.74	9 (17%)
5	CHL	C	312	10	62,74,74	4.78	20 (32%)	52,114,114	1.68	12 (23%)
5	CHL	C	313	1	62,74,74	3.87	17 (27%)	52,114,114	1.84	13 (25%)
6	CLA	C	314	1	73,73,73	2.21	17 (23%)	96,113,113	2.23	28 (29%)
6	CLA	C	315	4	73,73,73	2.33	18 (24%)	96,113,113	2.19	26 (27%)
6	CLA	C	316	1	73,73,73	2.27	17 (23%)	96,113,113	2.08	27 (28%)
6	CLA	C	317	1	73,73,73	2.17	18 (24%)	96,113,113	2.19	30 (31%)
6	CLA	C	318	1	48,48,73	4.19	21 (43%)	60,82,113	2.42	20 (33%)
7	CAC	C	319	8	4,4,4	4.67	3 (75%)	6,6,6	25.36	4 (66%)

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	LUT	A	301	-	-	0/29/67/67	0/2/2/2
2	LUT	A	302	-	-	0/29/67/67	0/2/2/2
3	NEX	A	303	-	-	0/27/83/83	0/2/3/3
4	LHG	A	304	6	-	0/53/53/53	0/0/0/0
5	CHL	A	305	1	-	0/41/177/177	0/0/9/9
6	CLA	A	306	1	-	0/37/135/135	0/0/9/9
6	CLA	A	307	1	-	0/37/135/135	0/0/9/9
6	CLA	A	308	10	-	0/34/132/135	0/0/9/9
5	CHL	A	309	1	-	0/20/156/177	0/0/9/9
5	CHL	A	310	10	-	0/23/159/177	0/0/9/9
5	CHL	A	311	10	-	0/41/177/177	0/0/9/9
5	CHL	A	312	10	-	0/41/177/177	0/0/9/9
5	CHL	A	313	1	-	0/41/177/177	0/0/9/9
6	CLA	A	314	1	-	0/37/135/135	0/0/9/9
6	CLA	A	315	4	-	0/37/135/135	0/0/9/9
6	CLA	A	316	1	-	0/37/135/135	0/0/9/9
6	CLA	A	317	1	-	0/37/135/135	0/0/9/9
6	CLA	A	318	1	-	0/8/106/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CAC	A	319	8	-	0/0/0/0	0/0/0/0
2	LUT	B	301	-	-	0/29/67/67	0/2/2/2
2	LUT	B	302	-	-	0/29/67/67	0/2/2/2
3	NEX	B	303	-	-	0/27/83/83	0/2/3/3
4	LHG	B	304	6	-	0/53/53/53	0/0/0/0
5	CHL	B	305	1	-	0/41/177/177	0/0/9/9
6	CLA	B	306	1	-	0/37/135/135	0/0/9/9
6	CLA	B	307	1	-	0/37/135/135	0/0/9/9
6	CLA	B	308	10	-	0/34/132/135	0/0/9/9
5	CHL	B	309	1	-	0/20/156/177	0/0/9/9
5	CHL	B	310	10	-	0/23/159/177	0/0/9/9
5	CHL	B	311	10	-	0/41/177/177	0/0/9/9
5	CHL	B	312	10	-	0/41/177/177	0/0/9/9
5	CHL	B	313	1	-	0/41/177/177	0/0/9/9
6	CLA	B	314	1	-	0/37/135/135	0/0/9/9
6	CLA	B	315	4	-	0/37/135/135	0/0/9/9
6	CLA	B	316	1	-	0/37/135/135	0/0/9/9
6	CLA	B	317	1	-	0/37/135/135	0/0/9/9
6	CLA	B	318	1	-	0/8/106/135	0/0/9/9
7	CAC	B	319	8	-	0/0/0/0	0/0/0/0
2	LUT	C	301	-	-	0/29/67/67	0/2/2/2
2	LUT	C	302	-	-	0/29/67/67	0/2/2/2
3	NEX	C	303	-	-	0/27/83/83	0/2/3/3
4	LHG	C	304	6	-	0/53/53/53	0/0/0/0
5	CHL	C	305	1	-	0/41/177/177	0/0/9/9
6	CLA	C	306	1	-	0/37/135/135	0/0/9/9
6	CLA	C	307	1	-	0/37/135/135	0/0/9/9
6	CLA	C	308	10	-	0/34/132/135	0/0/9/9
5	CHL	C	309	1	-	0/20/156/177	0/0/9/9
5	CHL	C	310	10	-	0/23/159/177	0/0/9/9
5	CHL	C	311	10	-	0/41/177/177	0/0/9/9
5	CHL	C	312	10	-	0/41/177/177	0/0/9/9
5	CHL	C	313	1	-	0/41/177/177	0/0/9/9
6	CLA	C	314	1	-	0/37/135/135	0/0/9/9
6	CLA	C	315	4	-	0/37/135/135	0/0/9/9
6	CLA	C	316	1	-	0/37/135/135	0/0/9/9
6	CLA	C	317	1	-	0/37/135/135	0/0/9/9
6	CLA	C	318	1	-	0/8/102/135	0/0/9/9
7	CAC	C	319	8	-	0/0/0/0	0/0/0/0

The worst 5 of 802 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	311	CHL	C1A-CHA	25.24	1.51	1.39
5	A	305	CHL	C1A-CHA	23.87	1.50	1.39
5	A	313	CHL	C1A-CHA	23.39	1.50	1.39
5	C	312	CHL	C3B-C2B	-23.28	1.27	1.45
5	C	312	CHL	C1A-CHA	23.14	1.50	1.39

The worst 5 of 1025 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	319	CAC	O2-AS-O1	-56.08	100.44	112.54
7	B	319	CAC	O2-AS-O1	-53.64	100.97	112.54
7	A	319	CAC	O2-AS-O1	-35.35	104.91	112.54
7	A	319	CAC	O2-AS-C2	-27.19	86.90	109.15
7	C	319	CAC	O2-AS-C2	-26.21	87.70	109.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	208/224 (92%)	0.02	14 (6%) 17 15	6, 39, 77, 97	0
1	B	208/224 (92%)	-0.15	10 (4%) 29 26	8, 34, 67, 94	0
1	C	208/224 (92%)	-0.18	8 (3%) 38 35	6, 33, 69, 107	0
All	All	624/672 (92%)	-0.10	32 (5%) 11 23	6, 35, 70, 107	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	217	VAL	5.0
1	A	89	GLY	4.9
1	A	213	LEU	4.7
1	A	88	ASN	4.0
1	A	214	ALA	4.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	LHG	B	304	49/49	0.19	5.40	14,40,98,107	0
3	NEX	B	303	44/44	0.27	3.91	26,42,94,97	0
3	NEX	A	303	44/44	0.25	3.77	26,39,94,96	0
6	CLA	B	307	65/65	0.19	3.74	9,20,82,94	0
9	NA	C	323	1/1	0.29	3.67	68,68,68,68	0
9	NA	C	320	1/1	0.23	3.18	60,60,60,60	0
6	CLA	B	316	65/65	0.27	2.91	28,41,89,99	0
6	CLA	C	307	65/65	0.20	2.74	6,18,80,92	0
4	LHG	A	304	49/49	0.17	2.55	19,42,98,108	0
6	CLA	A	307	65/65	0.20	2.30	10,20,81,93	0
6	CLA	A	306	65/65	0.17	2.20	13,21,43,63	0
5	CHL	A	309	48/66	0.27	2.16	32,48,95,101	0
5	CHL	A	311	66/66	0.19	1.92	19,37,99,119	0
4	LHG	C	304	49/49	0.18	1.77	16,42,96,107	0
5	CHL	C	313	66/66	0.17	1.77	5,21,66,80	0
6	CLA	C	306	65/65	0.16	1.76	7,19,41,60	0
5	CHL	B	313	66/66	0.16	1.70	14,28,69,85	0
5	CHL	B	311	66/66	0.18	1.69	21,38,99,119	0
6	CLA	B	315	65/65	0.23	1.57	20,43,74,83	0
6	CLA	B	306	65/65	0.16	1.53	9,19,39,58	0
5	CHL	C	311	66/66	0.18	1.42	11,31,94,115	0
5	CHL	C	309	48/66	0.21	1.41	26,43,97,104	0
5	CHL	A	313	66/66	0.15	1.33	14,25,68,82	0
2	LUT	B	302	42/42	0.15	1.21	6,19,32,35	0
6	CLA	C	314	65/65	0.19	1.15	15,27,79,93	0
5	CHL	A	305	66/66	0.18	1.09	17,32,86,104	0
5	CHL	A	310	51/66	0.17	1.03	21,36,94,100	0
6	CLA	B	314	65/65	0.20	0.98	24,31,80,96	0
6	CLA	C	316	65/65	0.23	0.97	22,37,84,97	0
6	CLA	C	315	65/65	0.20	0.96	21,45,74,87	0
6	CLA	B	318	41/65	0.29	0.78	44,76,92,115	0
7	CAC	C	319	5/5	0.16	0.75	57,62,79,156	0
3	NEX	C	303	44/44	0.21	0.71	14,32,90,92	0
5	CHL	B	309	48/66	0.22	0.69	35,52,99,105	0
6	CLA	A	314	65/65	0.19	0.61	23,34,78,93	0
5	CHL	B	305	66/66	0.16	0.56	8,26,81,100	0
2	LUT	A	302	42/42	0.15	0.55	7,21,31,37	0
2	LUT	C	301	42/42	0.17	0.45	15,22,35,57	0
2	LUT	C	302	42/42	0.14	0.44	6,16,30,35	0
5	CHL	C	305	66/66	0.15	0.37	14,34,87,104	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CLA	A	318	41/65	0.34	0.34	44,79,96,119	0
6	CLA	A	315	65/65	0.20	0.20	28,48,76,86	0
6	CLA	A	316	65/65	0.22	0.18	30,41,88,98	0
5	CHL	B	312	66/66	0.16	0.13	22,40,71,83	0
6	CLA	B	308	62/65	0.17	0.08	21,37,83,91	0
6	CLA	C	317	65/65	0.15	0.08	16,31,87,95	0
5	CHL	C	312	66/66	0.17	0.05	9,32,66,79	0
6	CLA	C	308	62/65	0.15	0.02	12,28,80,87	0
6	CLA	C	318	40/65	0.24	0.01	36,69,91,110	0
5	CHL	A	312	66/66	0.14	-0.06	19,36,68,81	0
5	CHL	B	310	51/66	0.13	-0.07	20,32,92,97	0
6	CLA	B	317	65/65	0.16	-0.07	14,30,85,94	0
6	CLA	A	317	65/65	0.18	-0.10	21,37,90,99	0
6	CLA	A	308	62/65	0.17	-0.20	20,35,82,89	0
2	LUT	B	301	42/42	0.14	-0.23	18,26,42,62	0
5	CHL	C	310	51/66	0.12	-0.23	13,27,89,94	0
2	LUT	A	301	42/42	0.16	-0.33	20,25,39,61	0
8	ZN	C	321	1/1	0.13	-0.48	64,64,64,64	0
7	CAC	A	319	5/5	0.15	-0.49	57,59,68,81	0
9	NA	B	322	1/1	0.14	-0.63	47,47,47,47	0
7	CAC	B	319	5/5	0.13	-0.84	59,62,68,97	0
8	ZN	A	320	1/1	0.12	-0.86	98,98,98,98	0
8	ZN	B	321	1/1	0.10	-1.19	66,66,66,66	0
8	ZN	A	321	1/1	0.08	-1.45	56,56,56,56	0
8	ZN	A	322	1/1	0.23	-3.34	122,122,122,122	0
9	NA	B	320	1/1	0.07	-3.81	42,42,42,42	0
9	NA	C	322	1/1	0.39	-	80,80,80,80	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.