



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:30 PM GMT

PDB ID : 1KMO  
Title : Crystal structure of the Outer Membrane Transporter FecA  
Authors : Ferguson, A.D.; Chakraborty, R.; Smith, B.S.; Esser, L.; van der Helm, D.;  
Deisenhofer, J.  
Deposited on : 2001-12-17  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

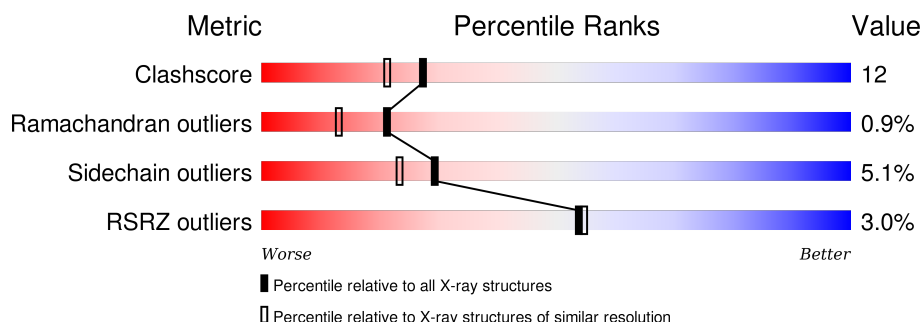
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	774	

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	742	-	-	-	X
2	LDA	A	743	-	-	-	X
2	LDA	A	744	-	-	-	X
2	LDA	A	745	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LDA	A	746	-	-	-	X
2	LDA	A	747	-	-	-	X
2	LDA	A	748	-	-	-	X
2	LDA	A	749	-	-	-	X
2	LDA	A	750	-	-	-	X
2	LDA	A	751	-	-	-	X
2	LDA	A	753	-	-	-	X
2	LDA	A	754	-	-	-	X
2	LDA	A	755	-	-	-	X
2	LDA	A	756	-	-	-	X
2	LDA	A	757	-	-	-	X
2	LDA	A	758	-	-	-	X
3	HTO	A	759	-	-	-	X
3	HTO	A	760	-	-	-	X

## 2 Entry composition [i](#)

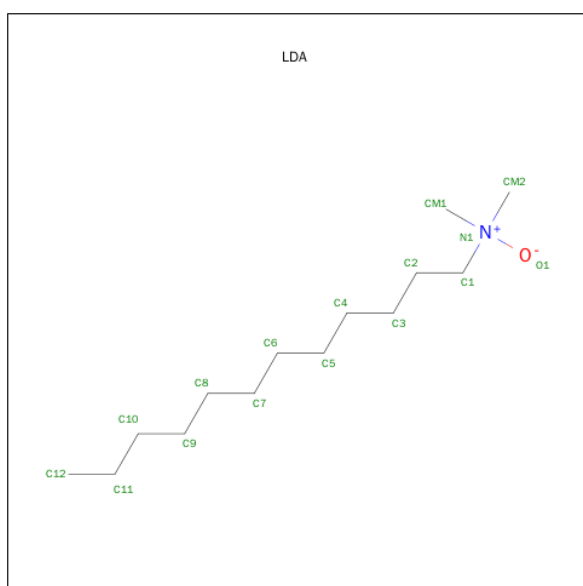
There are 4 unique types of molecules in this entry. The entry contains 5862 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Iron(III) dicitrate transport protein fecA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	0	0
			5184	3244	912	1014	14			

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



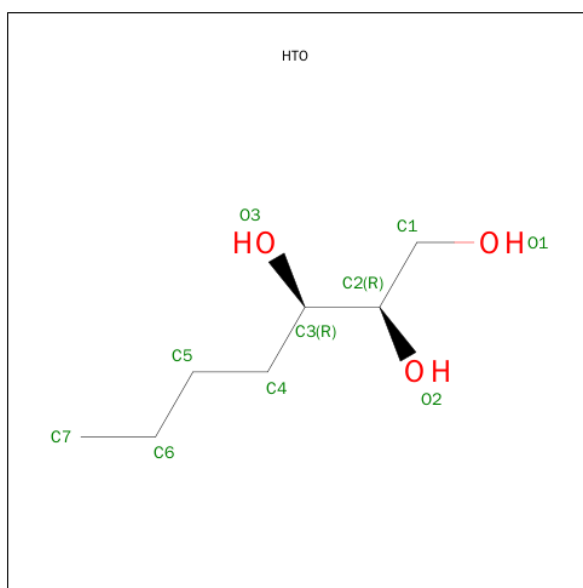
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		

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

- Molecule 3 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula:  $C_7H_{16}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	7	3		
3	A	1	Total	C	O	0	0
			10	7	3		

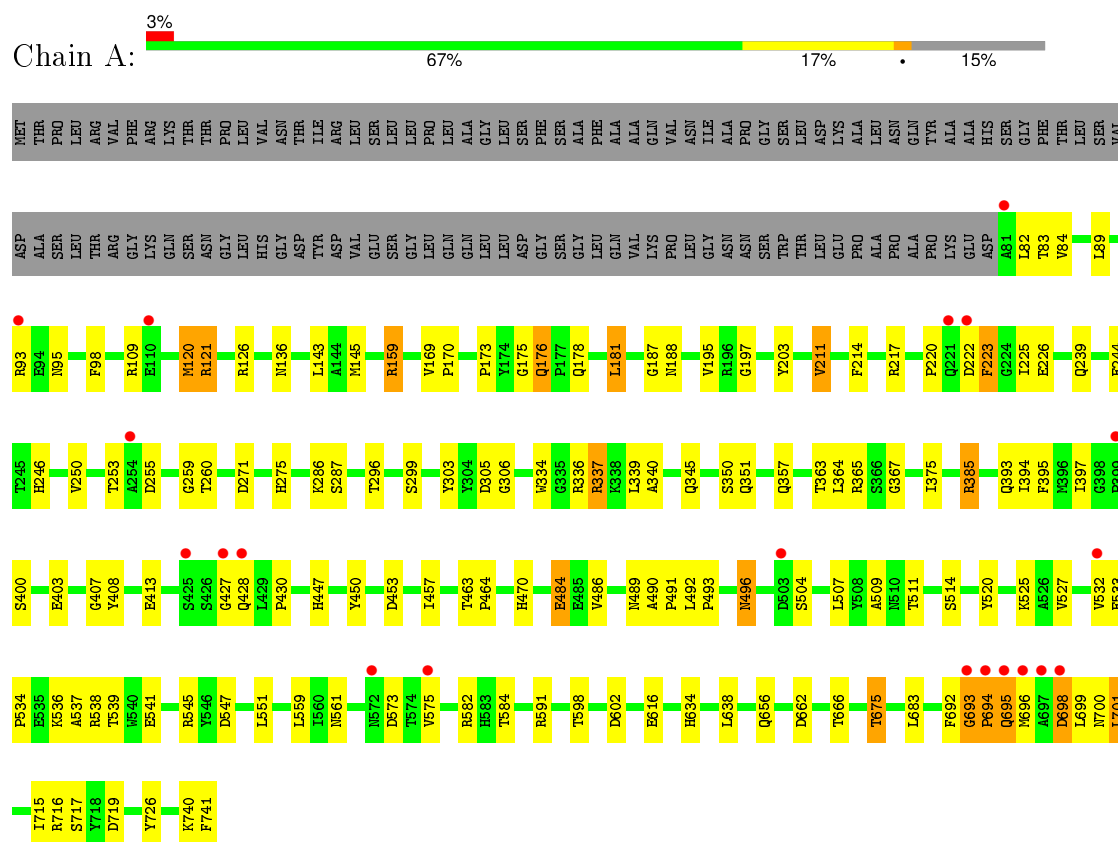
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	386	Total	O	0	0
			386	386		

### 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: Iron(III) dicitrate transport protein fecA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.08 Å 88.09 Å 94.58 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.71 – 2.00 19.71 – 1.94	Depositor EDS
% Data completeness (in resolution range)	84.5 (19.71-2.00) 82.6 (19.71-1.94)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 1.94 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.207 , 0.245 0.212 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 62.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 67469 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5862	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: HTO, LDA

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	0.57	0/5315	0.81	4/7220 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	427	GLY	N-CA-C	-6.55	96.71	113.10
1	A	121	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	337	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	717	SER	N-CA-C	-5.15	97.10	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	5184	0	4898	129	0
2	A	272	0	527	11	0
3	A	20	0	32	0	0
4	A	386	0	0	18	0
All	All	5862	0	5457	130	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 12.

All (130) 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:A:159:ARG:HH11	1:A:159:ARG:HG2	1.09	1.14
1:A:226:GLU:HG2	1:A:740:LYS:HG2	1.47	0.96
1:A:533:GLU:HG3	1:A:534:PRO:HD2	1.54	0.89
1:A:385:ARG:HH11	1:A:385:ARG:HB3	1.40	0.85
1:A:159:ARG:NH1	1:A:159:ARG:HG2	1.91	0.84
1:A:159:ARG:CG	1:A:159:ARG:HH11	1.92	0.82
1:A:701:LEU:HD13	2:A:745:LDA:HM11	1.60	0.82
1:A:176:GLN:NE2	1:A:178:GLN:OE1	2.13	0.82
1:A:195:VAL:HB	1:A:211:VAL:HG13	1.61	0.81
1:A:692:PHE:CD1	1:A:699:LEU:HD12	2.23	0.72
1:A:699:LEU:HD13	1:A:699:LEU:C	2.11	0.71
1:A:225:ILE:HG12	1:A:250:VAL:HG12	1.72	0.70
1:A:159:ARG:NH1	4:A:1013:HOH:O	2.24	0.69
1:A:296:THR:OG1	1:A:345:GLN:HB3	1.93	0.69
1:A:699:LEU:HD13	1:A:700:ASN:N	2.10	0.66
1:A:692:PHE:HD1	1:A:699:LEU:HD12	1.60	0.65
1:A:176:GLN:C	1:A:176:GLN:HE21	2.00	0.65
1:A:692:PHE:O	1:A:693:GLY:C	2.35	0.65
1:A:463:THR:HB	1:A:496:ASN:ND2	2.13	0.64
1:A:715:ILE:HG12	1:A:716:ARG:N	2.13	0.64
1:A:533:GLU:HG2	1:A:536:LYS:NZ	2.14	0.63
1:A:662:ASP:OD2	1:A:666:THR:HG23	1.99	0.62
1:A:490:ALA:O	1:A:492:LEU:HD22	1.99	0.62
1:A:239:GLN:HG2	1:A:271:ASP:O	2.00	0.62
1:A:350:SER:OG	1:A:351:GLN:NE2	2.33	0.62
1:A:463:THR:HB	1:A:496:ASN:HD21	1.66	0.61
1:A:715:ILE:HG12	1:A:716:ARG:H	1.66	0.60
1:A:698:ASP:HB2	1:A:740:LYS:HB2	1.83	0.60
1:A:120:MET:HG2	1:A:145:MET:HE1	1.83	0.60
1:A:339:LEU:C	1:A:339:LEU:HD23	2.22	0.60
1:A:176:GLN:CA	1:A:176:GLN:HE21	2.15	0.59
1:A:693:GLY:O	1:A:695:GLN:N	2.37	0.58
1:A:385:ARG:NH1	1:A:385:ARG:HB3	2.17	0.58
1:A:693:GLY:O	1:A:695:GLN:O	2.22	0.58
1:A:176:GLN:HE22	1:A:178:GLN:HB2	1.69	0.58
1:A:220:PRO:O	1:A:253:THR:HG23	2.04	0.57
1:A:303:TYR:OH	1:A:336:ARG:NH1	2.39	0.56
1:A:175:GLY:HA3	1:A:520:TYR:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ASN:HB3	4:A:1058:HOH:O	2.05	0.56
1:A:470:HIS:ND1	1:A:489:ASN:ND2	2.53	0.56
1:A:457:ILE:HG23	1:A:457:ILE:O	2.05	0.56
1:A:84:VAL:N	1:A:394:ILE:HD13	2.21	0.55
1:A:493:PRO:HB3	2:A:755:LDA:HM21	1.89	0.55
1:A:453:ASP:O	1:A:464:PRO:HD2	2.07	0.54
1:A:509:ALA:HB2	2:A:754:LDA:HM23	1.89	0.54
1:A:699:LEU:CD1	1:A:699:LEU:C	2.76	0.53
1:A:491:PRO:O	1:A:492:LEU:HD13	2.08	0.53
1:A:126:ARG:HD3	4:A:878:HOH:O	2.08	0.53
1:A:395:PHE:HE1	1:A:397:ILE:HD11	1.72	0.53
1:A:188:ASN:O	1:A:217:ARG:HG2	2.08	0.53
1:A:260:THR:HG22	1:A:287:SER:OG	2.10	0.52
1:A:83:THR:C	1:A:394:ILE:HD13	2.30	0.52
1:A:287:SER:HB2	1:A:299:SER:OG	2.10	0.52
1:A:538:ARG:HD3	2:A:749:LDA:HM13	1.92	0.52
1:A:486:VAL:HB	1:A:532:VAL:HG11	1.93	0.51
1:A:533:GLU:CG	1:A:534:PRO:HD2	2.33	0.50
1:A:95:ASN:N	1:A:95:ASN:HD22	2.08	0.50
1:A:545:ARG:HG3	1:A:545:ARG:HH11	1.77	0.49
1:A:296:THR:HG1	1:A:345:GLN:HB3	1.76	0.49
1:A:98:PHE:CD1	1:A:545:ARG:HD2	2.48	0.49
1:A:375:ILE:O	1:A:430:PRO:HG3	2.13	0.48
1:A:533:GLU:HG3	1:A:536:LYS:HE2	1.95	0.48
1:A:175:GLY:HA3	1:A:520:TYR:CZ	2.48	0.48
1:A:250:VAL:HG23	1:A:250:VAL:O	2.13	0.48
1:A:675:THR:HG21	4:A:1080:HOH:O	2.12	0.48
1:A:538:ARG:HD2	4:A:1070:HOH:O	2.13	0.48
1:A:470:HIS:HA	1:A:489:ASN:HD22	1.79	0.48
1:A:143:LEU:HD21	1:A:306:GLY:C	2.34	0.47
1:A:246:HIS:HB2	2:A:742:LDA:H61	1.96	0.47
1:A:176:GLN:HG2	4:A:813:HOH:O	2.14	0.47
1:A:169:VAL:N	1:A:170:PRO:CD	2.78	0.47
1:A:136:ASN:HA	1:A:726:TYR:CE2	2.50	0.47
1:A:394:ILE:HG22	1:A:403:GLU:CB	2.45	0.47
1:A:533:GLU:HG2	1:A:536:LYS:HZ1	1.79	0.46
1:A:159:ARG:NH1	1:A:159:ARG:CG	2.62	0.46
1:A:695:GLN:HE21	1:A:695:GLN:HB3	1.51	0.46
1:A:504:SER:HB2	1:A:547:ASP:O	2.15	0.46
1:A:582:ARG:NH1	1:A:616:GLU:OE2	2.49	0.46
1:A:545:ARG:NH1	4:A:1017:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ARG:NE	4:A:961:HOH:O	2.48	0.46
1:A:159:ARG:NH2	4:A:1013:HOH:O	2.47	0.46
1:A:394:ILE:HG22	1:A:403:GLU:HB2	1.98	0.46
1:A:525:LYS:NZ	1:A:573:ASP:OD1	2.49	0.45
1:A:693:GLY:C	1:A:695:GLN:N	2.69	0.45
1:A:511:THR:HA	1:A:539:THR:O	2.16	0.45
1:A:408:TYR:HB3	2:A:751:LDA:H92	1.99	0.45
1:A:275:HIS:HE1	4:A:936:HOH:O	1.99	0.45
1:A:400:SER:HB3	1:A:457:ILE:HD13	1.99	0.45
1:A:447:HIS:HE1	2:A:750:LDA:H123	1.82	0.45
1:A:226:GLU:OE1	1:A:740:LYS:HE2	2.17	0.45
1:A:741:PHE:CG	2:A:747:LDA:H52	2.52	0.45
1:A:159:ARG:CD	4:A:861:HOH:O	2.64	0.44
1:A:181:LEU:HD12	1:A:363:THR:CG2	2.48	0.44
1:A:634:HIS:O	1:A:656:GLN:HA	2.18	0.44
1:A:89:LEU:HD22	1:A:203:TYR:CZ	2.53	0.44
1:A:253:THR:HA	1:A:259:GLY:HA2	2.00	0.43
1:A:559:LEU:HD13	1:A:584:THR:HG22	1.99	0.43
1:A:260:THR:HG22	1:A:287:SER:CB	2.48	0.43
1:A:197:GLY:HA3	1:A:541:GLU:OE1	2.19	0.43
1:A:351:GLN:O	1:A:393:GLN:HA	2.19	0.43
1:A:305:ASP:OD1	1:A:336:ARG:CZ	2.66	0.43
1:A:176:GLN:NE2	1:A:176:GLN:CA	2.79	0.43
1:A:159:ARG:NH2	4:A:961:HOH:O	2.51	0.42
1:A:715:ILE:HD11	4:A:930:HOH:O	2.18	0.42
1:A:334:TRP:CZ3	1:A:367:GLY:HA2	2.55	0.42
1:A:305:ASP:OD1	1:A:336:ARG:NH2	2.53	0.42
1:A:533:GLU:CG	1:A:536:LYS:NZ	2.82	0.42
1:A:159:ARG:CZ	4:A:1013:HOH:O	2.65	0.42
1:A:173:PRO:HD2	1:A:413:GLU:OE1	2.20	0.42
1:A:336:ARG:HH22	2:A:743:LDA:H123	1.85	0.42
1:A:695:GLN:O	1:A:696:MET:HB3	2.19	0.42
1:A:407:GLY:HA3	1:A:450:TYR:CE2	2.55	0.41
1:A:159:ARG:HD3	4:A:861:HOH:O	2.19	0.41
1:A:109:ARG:NH2	1:A:187:GLY:O	2.53	0.41
1:A:591:ARG:NH2	4:A:1135:HOH:O	2.53	0.41
1:A:339:LEU:HD23	1:A:340:ALA:N	2.36	0.41
1:A:98:PHE:HA	1:A:545:ARG:HD2	2.01	0.41
1:A:93:ARG:HG2	1:A:93:ARG:HH11	1.86	0.41
1:A:484:GLU:HG2	1:A:527:VAL:HG21	2.03	0.41
1:A:701:LEU:HD13	2:A:745:LDA:CM1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ARG:CD	4:A:878:HOH:O	2.66	0.41
1:A:217:ARG:HG2	1:A:217:ARG:H	1.63	0.41
1:A:226:GLU:HG2	1:A:740:LYS:CG	2.34	0.41
1:A:222:ASP:O	1:A:223:PHE:C	2.59	0.41
1:A:395:PHE:HE1	1:A:397:ILE:CD1	2.33	0.40
1:A:120:MET:HG3	1:A:214:PHE:CE1	2.56	0.40
1:A:260:THR:HA	1:A:286:LYS:O	2.20	0.40
1:A:93:ARG:HG2	1:A:93:ARG:NH1	2.37	0.40
1:A:537:ALA:HA	1:A:561:ASN:O	2.22	0.40
2:A:743:LDA:H82	4:A:1118:HOH:O	2.22	0.40

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	659/774 (85%)	638 (97%)	15 (2%)	6 (1%)	21 13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	LEU
1	A	428	GLN
1	A	223	PHE
1	A	693	GLY
1	A	694	PRO
1	A	698	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	544/636 (86%)	516 (95%)	28 (5%)	29	23

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	MET
1	A	121	ARG
1	A	159	ARG
1	A	176	GLN
1	A	181	LEU
1	A	211	VAL
1	A	244	GLU
1	A	255	ASP
1	A	337	ARG
1	A	357	GLN
1	A	364	LEU
1	A	365	ARG
1	A	385	ARG
1	A	484	GLU
1	A	496	ASN
1	A	507	LEU
1	A	514	SER
1	A	551	LEU
1	A	575	VAL
1	A	598	THR
1	A	602	ASP
1	A	638	LEU
1	A	675	THR
1	A	683	LEU
1	A	694	PRO
1	A	695	GLN
1	A	701	LEU
1	A	719	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	176	GLN
1	A	240	ASN
1	A	275	HIS
1	A	351	GLN
1	A	489	ASN
1	A	496	ASN
1	A	563	ASN
1	A	652	ASN
1	A	695	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

19 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	LDA	A	742	-	15,15,15	3.89	2 (13%)	16,17,17	2.61	4 (25%)
2	LDA	A	743	-	15,15,15	3.94	2 (13%)	16,17,17	2.64	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LDA	A	744	-	15,15,15	3.98	2 (13%)	16,17,17	2.56	3 (18%)
2	LDA	A	745	-	15,15,15	4.27	2 (13%)	16,17,17	2.45	3 (18%)
2	LDA	A	746	-	15,15,15	3.91	2 (13%)	16,17,17	2.67	4 (25%)
2	LDA	A	747	-	15,15,15	3.93	2 (13%)	16,17,17	2.56	4 (25%)
2	LDA	A	748	-	15,15,15	4.02	2 (13%)	16,17,17	2.52	3 (18%)
2	LDA	A	749	-	15,15,15	3.92	2 (13%)	16,17,17	2.59	4 (25%)
2	LDA	A	750	-	15,15,15	3.86	2 (13%)	16,17,17	2.61	5 (31%)
2	LDA	A	751	-	15,15,15	3.93	2 (13%)	16,17,17	2.58	5 (31%)
2	LDA	A	752	-	15,15,15	3.90	2 (13%)	16,17,17	2.69	4 (25%)
2	LDA	A	753	-	15,15,15	3.89	2 (13%)	16,17,17	2.57	4 (25%)
2	LDA	A	754	-	15,15,15	3.83	2 (13%)	16,17,17	2.64	4 (25%)
2	LDA	A	755	-	15,15,15	4.09	2 (13%)	16,17,17	2.52	4 (25%)
2	LDA	A	756	-	15,15,15	3.75	2 (13%)	16,17,17	2.68	4 (25%)
2	LDA	A	757	-	15,15,15	4.04	2 (13%)	16,17,17	2.54	4 (25%)
2	LDA	A	758	-	15,15,15	3.80	2 (13%)	16,17,17	2.65	4 (25%)
3	HTO	A	759	-	9,9,9	1.23	1 (11%)	8,10,10	0.38	0
3	HTO	A	760	-	9,9,9	1.42	1 (11%)	8,10,10	0.48	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
2	LDA	A	742	-	-	0/13/13/13	0/0/0/0
2	LDA	A	743	-	-	0/13/13/13	0/0/0/0
2	LDA	A	744	-	-	0/13/13/13	0/0/0/0
2	LDA	A	745	-	-	0/13/13/13	0/0/0/0
2	LDA	A	746	-	-	0/13/13/13	0/0/0/0
2	LDA	A	747	-	-	0/13/13/13	0/0/0/0
2	LDA	A	748	-	-	0/13/13/13	0/0/0/0
2	LDA	A	749	-	-	0/13/13/13	0/0/0/0
2	LDA	A	750	-	-	0/13/13/13	0/0/0/0
2	LDA	A	751	-	-	0/13/13/13	0/0/0/0
2	LDA	A	752	-	-	0/13/13/13	0/0/0/0
2	LDA	A	753	-	-	0/13/13/13	0/0/0/0
2	LDA	A	754	-	-	0/13/13/13	0/0/0/0
2	LDA	A	755	-	-	0/13/13/13	0/0/0/0
2	LDA	A	756	-	-	0/13/13/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LDA	A	757	-	-	0/13/13/13	0/0/0/0
2	LDA	A	758	-	-	0/13/13/13	0/0/0/0
3	HTO	A	759	-	-	0/10/10/10	0/0/0/0
3	HTO	A	760	-	-	0/10/10/10	0/0/0/0

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	745	LDA	O1-N1	-15.61	1.24	1.39
2	A	755	LDA	O1-N1	-15.13	1.25	1.39
2	A	757	LDA	O1-N1	-14.91	1.25	1.39
2	A	748	LDA	O1-N1	-14.80	1.25	1.39
2	A	744	LDA	O1-N1	-14.62	1.25	1.39
2	A	751	LDA	O1-N1	-14.59	1.25	1.39
2	A	743	LDA	O1-N1	-14.56	1.25	1.39
2	A	747	LDA	O1-N1	-14.55	1.25	1.39
2	A	749	LDA	O1-N1	-14.50	1.25	1.39
2	A	746	LDA	O1-N1	-14.40	1.25	1.39
2	A	753	LDA	O1-N1	-14.36	1.25	1.39
2	A	742	LDA	O1-N1	-14.30	1.26	1.39
2	A	752	LDA	O1-N1	-14.23	1.26	1.39
2	A	750	LDA	O1-N1	-14.16	1.26	1.39
2	A	754	LDA	O1-N1	-14.00	1.26	1.39
2	A	758	LDA	O1-N1	-13.96	1.26	1.39
2	A	756	LDA	O1-N1	-13.77	1.26	1.39
2	A	745	LDA	CM2-N1	-4.79	1.42	1.49
2	A	752	LDA	CM2-N1	-4.26	1.42	1.49
2	A	744	LDA	CM2-N1	-4.23	1.42	1.49
2	A	750	LDA	CM2-N1	-4.15	1.43	1.49
2	A	754	LDA	CM2-N1	-4.13	1.43	1.49
2	A	757	LDA	CM2-N1	-4.12	1.43	1.49
2	A	748	LDA	CM2-N1	-4.00	1.43	1.49
2	A	755	LDA	CM2-N1	-3.92	1.43	1.49
2	A	742	LDA	CM2-N1	-3.90	1.43	1.49
2	A	758	LDA	CM2-N1	-3.89	1.43	1.49
2	A	743	LDA	CM2-N1	-3.86	1.43	1.49
2	A	746	LDA	CM2-N1	-3.85	1.43	1.49
2	A	756	LDA	CM2-N1	-3.84	1.43	1.49
2	A	753	LDA	CM2-N1	-3.84	1.43	1.49
2	A	751	LDA	CM2-N1	-3.80	1.43	1.49
2	A	749	LDA	CM2-N1	-3.77	1.43	1.49
2	A	747	LDA	CM2-N1	-3.74	1.43	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	759	HTO	C3-C2	2.82	1.60	1.52
3	A	760	HTO	C3-C2	3.18	1.61	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	752	LDA	CM2-N1-CM1	-8.12	99.67	108.83
2	A	746	LDA	CM2-N1-CM1	-8.07	99.73	108.83
2	A	744	LDA	CM2-N1-CM1	-7.80	100.03	108.83
2	A	756	LDA	CM2-N1-CM1	-7.77	100.06	108.83
2	A	742	LDA	CM2-N1-CM1	-7.75	100.08	108.83
2	A	750	LDA	CM2-N1-CM1	-7.67	100.18	108.83
2	A	749	LDA	CM2-N1-CM1	-7.64	100.22	108.83
2	A	743	LDA	CM2-N1-CM1	-7.62	100.23	108.83
2	A	747	LDA	CM2-N1-CM1	-7.61	100.25	108.83
2	A	757	LDA	CM2-N1-CM1	-7.60	100.25	108.83
2	A	755	LDA	CM2-N1-CM1	-7.59	100.27	108.83
2	A	753	LDA	CM2-N1-CM1	-7.51	100.35	108.83
2	A	751	LDA	CM2-N1-CM1	-7.46	100.41	108.83
2	A	754	LDA	CM2-N1-CM1	-7.46	100.41	108.83
2	A	758	LDA	CM2-N1-CM1	-7.42	100.46	108.83
2	A	748	LDA	CM2-N1-CM1	-7.39	100.49	108.83
2	A	745	LDA	CM2-N1-CM1	-7.19	100.72	108.83
2	A	756	LDA	C9-C8-C7	-2.36	102.33	114.53
2	A	750	LDA	C9-C8-C7	-2.32	102.55	114.53
2	A	751	LDA	C9-C8-C7	-2.32	102.56	114.53
2	A	746	LDA	C9-C8-C7	-2.32	102.57	114.53
2	A	756	LDA	CM1-N1-C1	-2.30	102.35	109.77
2	A	744	LDA	C9-C8-C7	-2.30	102.68	114.53
2	A	742	LDA	CM1-N1-C1	-2.29	102.40	109.77
2	A	754	LDA	C9-C8-C7	-2.27	102.80	114.53
2	A	758	LDA	CM1-N1-C1	-2.27	102.47	109.77
2	A	755	LDA	C9-C8-C7	-2.26	102.88	114.53
2	A	743	LDA	C9-C8-C7	-2.26	102.88	114.53
2	A	757	LDA	C9-C8-C7	-2.25	102.91	114.53
2	A	745	LDA	C9-C8-C7	-2.24	102.98	114.53
2	A	749	LDA	C9-C8-C7	-2.24	102.99	114.53
2	A	742	LDA	C9-C8-C7	-2.22	103.05	114.53
2	A	758	LDA	C9-C8-C7	-2.22	103.07	114.53
2	A	748	LDA	C9-C8-C7	-2.20	103.15	114.53
2	A	753	LDA	C9-C8-C7	-2.18	103.28	114.53
2	A	751	LDA	CM1-N1-C1	-2.17	102.77	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	LDA	CM1-N1-C1	-2.17	102.77	109.77
2	A	754	LDA	CM1-N1-C1	-2.15	102.84	109.77
2	A	743	LDA	CM1-N1-C1	-2.15	102.86	109.77
2	A	752	LDA	CM1-N1-C1	-2.14	102.89	109.77
2	A	752	LDA	C9-C8-C7	-2.13	103.53	114.53
2	A	753	LDA	CM1-N1-C1	-2.12	102.95	109.77
2	A	747	LDA	C9-C8-C7	-2.06	103.89	114.53
2	A	751	LDA	C6-C5-C4	-2.05	103.93	114.53
2	A	747	LDA	CM1-N1-C1	-2.05	103.16	109.77
2	A	755	LDA	CM1-N1-C1	-2.04	103.20	109.77
2	A	746	LDA	CM1-N1-C1	-2.03	103.23	109.77
2	A	757	LDA	CM1-N1-C1	-2.02	103.25	109.77
2	A	749	LDA	CM1-N1-C1	-2.02	103.28	109.77
2	A	750	LDA	C6-C5-C4	-2.00	104.18	114.53
2	A	744	LDA	O1-N1-C1	4.72	115.58	110.27
2	A	757	LDA	O1-N1-C1	4.77	115.64	110.27
2	A	755	LDA	O1-N1-C1	4.77	115.64	110.27
2	A	742	LDA	O1-N1-C1	4.85	115.73	110.27
2	A	745	LDA	O1-N1-C1	4.95	115.84	110.27
2	A	746	LDA	O1-N1-C1	5.01	115.91	110.27
2	A	751	LDA	O1-N1-C1	5.03	115.93	110.27
2	A	752	LDA	O1-N1-C1	5.07	115.98	110.27
2	A	750	LDA	O1-N1-C1	5.09	116.00	110.27
2	A	747	LDA	O1-N1-C1	5.14	116.06	110.27
2	A	748	LDA	O1-N1-C1	5.14	116.06	110.27
2	A	749	LDA	O1-N1-C1	5.16	116.08	110.27
2	A	753	LDA	O1-N1-C1	5.24	116.17	110.27
2	A	743	LDA	O1-N1-C1	5.42	116.38	110.27
2	A	756	LDA	O1-N1-C1	5.51	116.47	110.27
2	A	754	LDA	O1-N1-C1	5.73	116.73	110.27
2	A	758	LDA	O1-N1-C1	5.87	116.88	110.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	742	LDA	1	0
2	A	743	LDA	2	0
2	A	745	LDA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	747	LDA	1	0
2	A	749	LDA	1	0
2	A	750	LDA	1	0
2	A	751	LDA	1	0
2	A	754	LDA	1	0
2	A	755	LDA	1	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 ⓘ

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	661/774 (85%)	-0.22	20 (3%) 54 55	13, 22, 39, 79	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	694	PRO	10.6
1	A	81	ALA	5.6
1	A	695	GLN	5.2
1	A	693	GLY	4.8
1	A	428	GLN	4.6
1	A	696	MET	3.4
1	A	221	GLN	3.4
1	A	697	ALA	2.9
1	A	254	ALA	2.7
1	A	532	VAL	2.6
1	A	572	ASN	2.6
1	A	503	ASP	2.6
1	A	110	GLU	2.6
1	A	427	GLY	2.5
1	A	93	ARG	2.5
1	A	575	VAL	2.3
1	A	399	PRO	2.2
1	A	698	ASP	2.1
1	A	222	ASP	2.1
1	A	425	SER	2.0

### 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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	LDA	A	746	16/16	0.58	0.37	26.66	71,72,75,75	0
2	LDA	A	758	16/16	0.55	0.41	25.97	76,77,80,80	0
2	LDA	A	755	16/16	0.47	0.33	21.16	64,71,74,74	0
2	LDA	A	749	16/16	0.65	0.33	20.06	58,62,67,67	0
2	LDA	A	756	16/16	0.61	0.37	15.38	59,62,67,67	0
2	LDA	A	744	16/16	0.64	0.31	14.11	66,69,73,73	0
2	LDA	A	753	16/16	0.45	0.51	12.95	81,82,85,85	0
2	LDA	A	757	16/16	0.62	0.43	10.45	74,75,79,79	0
2	LDA	A	754	16/16	0.77	0.36	8.60	66,67,68,69	0
2	LDA	A	750	16/16	0.58	0.32	7.65	57,62,71,72	0
3	HTO	A	760	10/10	0.68	0.28	7.11	67,67,69,71	0
2	LDA	A	747	16/16	0.53	0.32	7.10	80,81,84,84	0
2	LDA	A	748	16/16	0.72	0.29	6.32	64,65,67,67	0
3	HTO	A	759	10/10	0.47	0.33	5.25	60,62,63,65	0
2	LDA	A	751	16/16	0.67	0.28	4.49	56,64,75,75	0
2	LDA	A	742	16/16	0.64	0.26	4.20	53,64,72,72	0
2	LDA	A	745	16/16	0.58	0.38	3.94	66,70,72,72	0
2	LDA	A	743	16/16	0.74	0.23	2.64	60,62,67,67	0
2	LDA	A	752	16/16	0.76	0.30	-	85,85,85,86	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.