



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:00 PM GMT

PDB ID : 4B61  
Title : In meso structure of alginate transporter, AlgE, from *Pseudomonas aeruginosa*, PAO1. Crystal form 3.  
Authors : Tan, J.; Pye, V.E.; Aragao, D.; Caffrey, M.  
Deposited on : 2012-08-08  
Resolution : 2.40 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

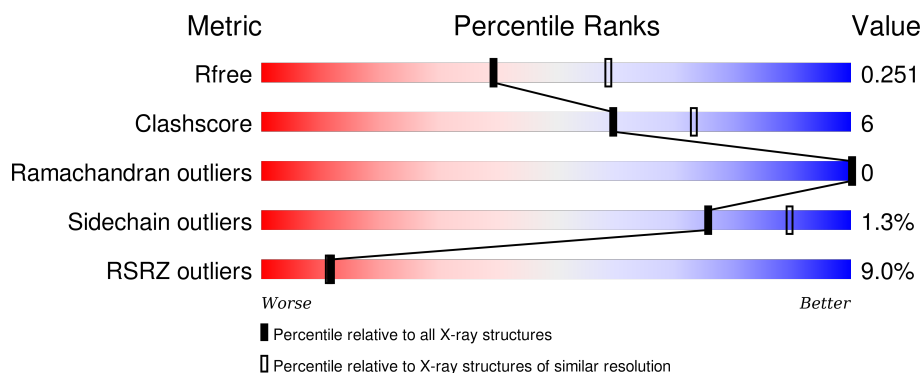
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	458	 8% 81% 12% 6%
1	B	458	 9% 83% 12% •

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	78M	A	1491	-	-	-	X
2	78M	A	1493	-	-	-	X
2	78M	A	1494	-	-	-	X
2	78M	A	1497	-	-	-	X
2	78M	A	1499	-	-	-	X
2	78M	A	1500	-	-	-	X
2	78M	B	1492	-	-	-	X
2	78M	B	1493	-	-	-	X
2	78M	B	1495	-	-	-	X
2	78M	B	1496	-	-	-	X
2	78M	B	1497	-	-	-	X
2	78M	B	1498	-	-	-	X
2	78M	B	1501	-	-	-	X
2	78M	B	1502	-	-	-	X
2	78M	B	1503	-	-	-	X
3	LDA	A	1502	-	-	-	X
6	78N	A	1506	-	-	-	X
6	78N	A	1507	-	-	-	X

## 2 Entry composition [i](#)

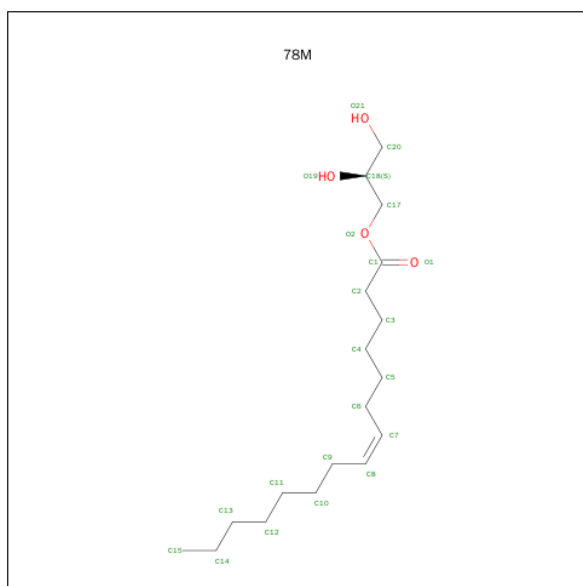
There are 8 unique types of molecules in this entry. The entry contains 7509 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALGINATE PRODUCTION PROTEIN ALGE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	4	0
			3433	2149	612	669	3			
1	B	439	Total	C	N	O	S	0	6	0
			3539	2214	628	693	4			

- Molecule 2 is (2S)-2,3-DIHYDROXYPROPYL(7Z)-PENTADEC-7-ENOATE (three-letter code: 78M) (formula: C<sub>18</sub>H<sub>34</sub>O<sub>4</sub>).



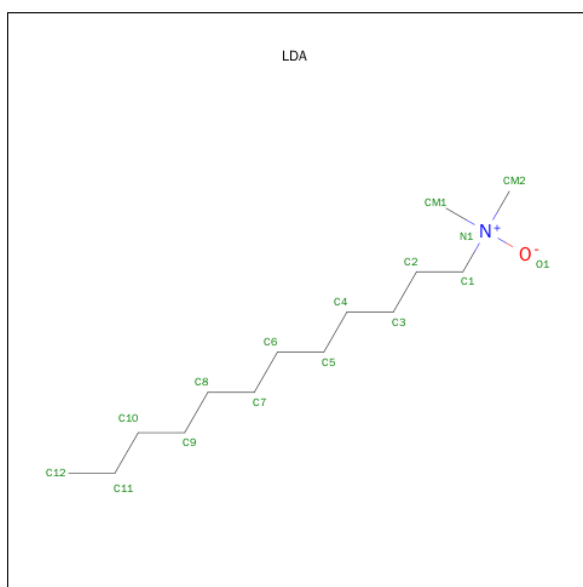
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			11	11		
2	A	1	Total	C	0	0
			15	15		
2	A	1	Total	C	0	0
			15	15		
2	A	1	Total	C	0	0
			11	11		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 11 11	0	0
2	A	1	Total C 11 11	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 8 8	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C O 22 18 4	0	0
2	B	1	Total C O 22 18 4	0	0
2	B	1	Total C O 22 18 4	0	0

- Molecule 3 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
3	A	1	Total	C	N	O	0	0
			16	14	1	1		

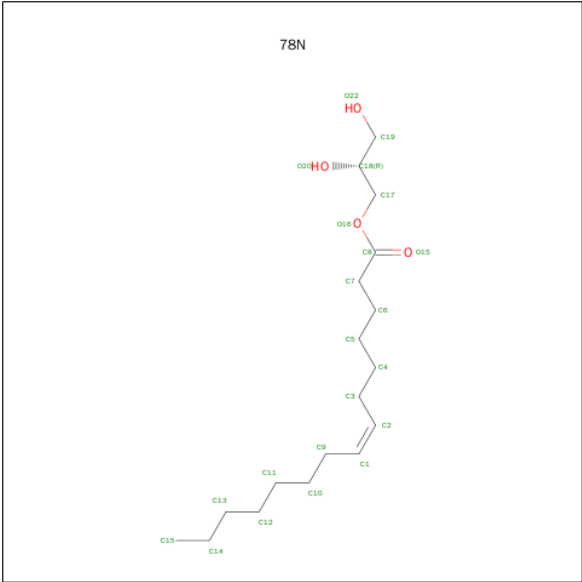
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

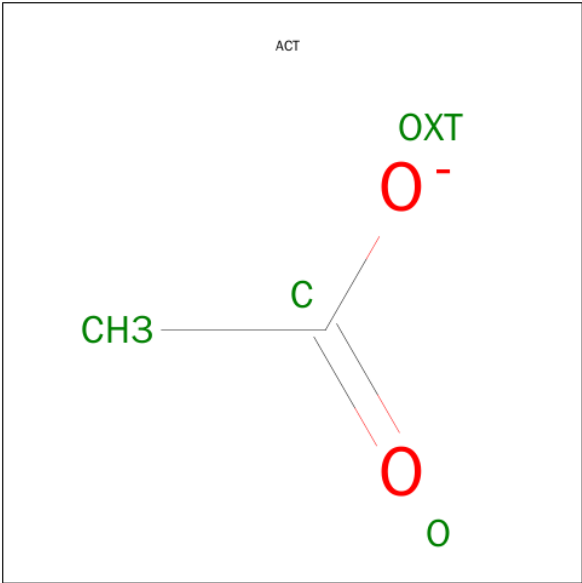
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Cu	0	0
			2	2		
5	A	2	Total	Cu	0	0
			2	2		

- Molecule 6 is (2R)-2,3-DIHYDROXYPROPYL(7Z)-PENTADEC-7-ENOATE (three-letter code: 78N) (formula: C<sub>18</sub>H<sub>34</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			22	18	4		
6	A	1	Total	C	O	0	0
			22	18	4		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

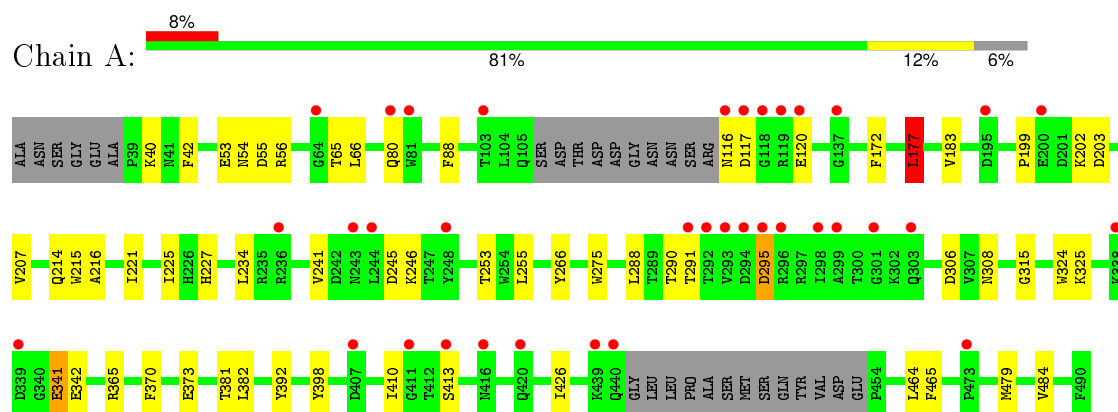
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	113	Total 113	O 113	0	0
8	B	91	Total 91	O 91	0	0



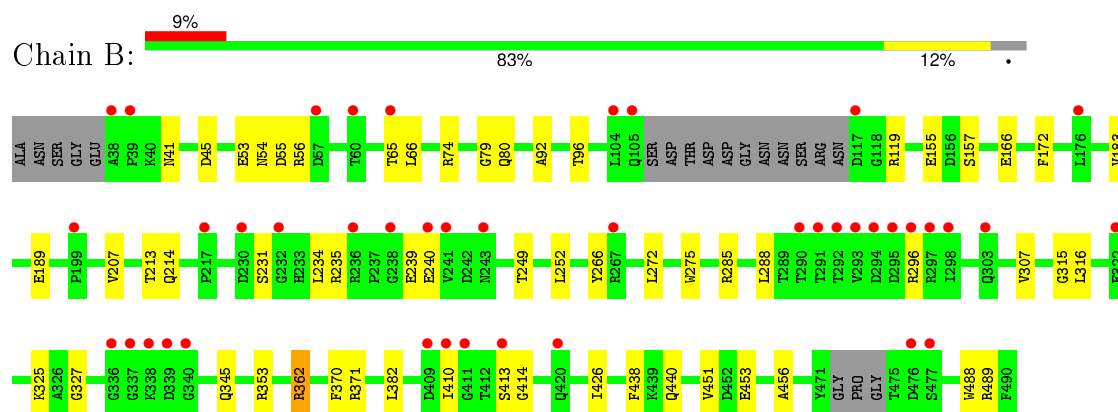
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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: ALGINATE PRODUCTION PROTEIN ALGE



#### • Molecule 1: ALGINATE PRODUCTION PROTEIN ALGE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.67Å 77.46Å 240.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.87 – 2.40 48.87 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.87-2.40) 99.3 (48.87-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.221 , 0.244 0.233 , 0.251	Depositor DCC
$R_{free}$ test set	2300 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.7	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.4	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	2 of 45614 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7509	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.61% 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: MG, LDA, ACT, 78M, 78N, CU

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	0.28	0/3528	0.56	1/4783 (0.0%)
1	B	0.25	0/3626	0.54	0/4918
All	All	0.26	0/7154	0.55	1/9701 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	LEU	CA-CB-CG	5.13	127.09	115.30

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	3433	0	3210	43	0
1	B	3539	0	3297	38	0
2	A	113	0	172	6	0
2	B	151	0	224	12	0
3	A	16	0	31	0	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	44	0	68	1	0
7	A	4	0	3	0	0
8	A	113	0	0	1	0
8	B	91	0	0	2	0
All	All	7509	0	7005	82	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 6.

All (82) 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:253:THR:HG21	2:B:1496:78M:H8	1.54	0.87
1:A:308:ASN:HB2	1:A:341:GLU:OE1	1.78	0.83
1:B:362:ARG:HD2	1:B:451:VAL:HG22	1.68	0.75
1:A:465:PHE:HB3	1:A:479:MET:HG3	1.71	0.71
1:B:453:GLU:O	1:B:489:ARG:NH2	2.23	0.71
1:B:119:ARG:NH2	1:B:189:GLU:OE2	2.27	0.67
1:B:285:ARG:NH2	1:B:345:GLN:OE1	2.28	0.66
1:B:183:VAL:HG12	1:B:207[B]:VAL:HG12	1.76	0.65
1:B:80:GLN:H	2:B:1503:78M:H201	1.62	0.64
1:B:213:THR:HB	2:B:1498:78M:H8	1.78	0.63
1:A:183:VAL:HG12	1:A:207[B]:VAL:HG22	1.83	0.60
1:A:410:ILE:HG21	1:A:426:ILE:HD11	1.85	0.59
1:A:365:ARG:HH12	1:A:381[A]:THR:HG21	1.67	0.58
1:A:199:PRO:O	1:A:246:LYS:NZ	2.30	0.57
1:A:88:PHE:HB2	2:A:1492:78M:H8	1.86	0.56
2:A:1494:78M:H61C	2:A:1496:78M:H62C	1.87	0.56
1:A:370:PHE:HZ	1:A:410:ILE:HD12	1.72	0.55
1:B:353:ARG:O	1:B:362:ARG:NH2	2.40	0.54
1:A:215:TRP:CZ3	2:B:1502:78M:H172	2.42	0.54
1:A:342:GLU:HG2	2:B:1501:78M:H202	1.90	0.53
1:B:45:ASP:HB2	1:B:74:ARG:HB2	1.91	0.53
1:A:382[B]:LEU:HD23	1:A:398:TYR:HD2	1.72	0.53
1:B:96:THR:HB	2:B:1501:78M:H18	1.91	0.53
1:B:410:ILE:HG21	1:B:426:ILE:HD11	1.92	0.52
1:B:362:ARG:NH2	8:B:2036:HOH:O	2.43	0.52
1:B:166:GLU:HB3	2:B:1492:78M:H22C	1.91	0.52
1:A:56:ARG:NH2	1:A:413:SER:O	2.42	0.52
1:B:240:GLU:HB2	1:B:296:ARG:HH21	1.75	0.52
1:B:55:ASP:HA	1:B:65:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:SER:HA	1:B:249:THR:HB	1.90	0.52
1:B:438:PHE:HB2	1:B:456:ALA:HB3	1.92	0.52
1:B:438:PHE:HB3	2:B:1502:78M:H18	1.93	0.51
1:A:306:ASP:O	1:A:341:GLU:HB2	2.10	0.51
1:B:41:ASN:ND2	8:B:2001:HOH:O	2.43	0.51
1:A:275:TRP:CZ2	1:A:315:GLY:HA3	2.46	0.50
1:A:373:GLU:OE2	1:A:413:SER:OG	2.30	0.50
1:B:370:PHE:HZ	1:B:410:ILE:HD12	1.77	0.49
1:A:221[B]:ILE:HD11	1:B:488:TRP:CZ2	2.47	0.49
1:B:53:GLU:HB3	1:B:66:LEU:HB2	1.94	0.49
1:A:214:GLN:HG2	1:A:216:ALA:O	2.13	0.49
2:A:1495:78M:H41C	2:A:1501:78M:H21C	1.95	0.48
1:B:275:TRP:CE2	1:B:315:GLY:HA3	2.48	0.48
1:A:266:TYR:O	1:A:325:LYS:NZ	2.43	0.48
1:B:272:LEU:HD21	1:B:316[A]:LEU:HD11	1.95	0.48
1:B:155:GLU:OE2	1:B:157:SER:OG	2.31	0.48
1:A:53:GLU:HB3	1:A:66:LEU:HB2	1.95	0.48
1:A:275:TRP:CE2	1:A:315:GLY:HA3	2.48	0.48
1:B:275:TRP:CZ2	1:B:315:GLY:HA3	2.48	0.48
1:A:116:ASN:O	1:A:120:GLU:HG3	2.14	0.47
1:B:79:GLY:HA3	2:B:1503:78M:H22C	1.97	0.47
1:A:234:LEU:HD22	1:A:288:LEU:HB2	1.97	0.47
1:A:40:LYS:HE2	1:A:42:PHE:O	2.15	0.46
1:A:382[B]:LEU:HD23	1:A:398:TYR:CD2	2.50	0.46
1:B:266:TYR:O	1:B:325:LYS:NZ	2.46	0.45
1:A:484:VAL:HG23	2:A:1499:78M:H52C	1.99	0.45
1:B:234:LEU:HD22	1:B:288:LEU:HB2	1.99	0.45
1:B:235:ARG:HD3	1:B:235:ARG:HA	1.83	0.45
1:A:308:ASN:O	2:B:1501:78M:O19	2.26	0.44
1:A:225:ILE:HD12	1:A:255:LEU:HD21	1.99	0.44
1:A:241:VAL:HG23	1:A:245:ASP:HB2	1.99	0.44
1:A:202:LYS:NZ	1:A:203:ASP:OD2	2.48	0.44
1:A:324:TRP:CD2	2:A:1494:78M:H51C	2.53	0.43
1:B:327:GLY:O	1:B:382:LEU:HD12	2.18	0.43
1:A:295:ASP:OD1	1:A:295:ASP:N	2.48	0.43
1:B:54:ASN:HA	1:B:65:THR:HG22	2.00	0.43
1:B:371:ARG:HB3	1:B:413:SER:HB2	2.01	0.43
1:A:215:TRP:CE3	2:B:1502:78M:H172	2.53	0.42
1:A:54:ASN:HA	1:A:65:THR:HG22	2.01	0.42
1:A:54:ASN:HA	1:A:55:ASP:HA	1.79	0.42
1:B:252:LEU:CD2	1:B:307:VAL:HG21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207[A]:VAL:HG13	1:A:227:HIS:HB3	2.02	0.41
1:A:55:ASP:HA	1:A:65:THR:HG22	2.01	0.41
1:B:234:LEU:HG	1:B:249:THR:HG23	2.01	0.41
1:A:172:PHE:CE1	1:A:177:LEU:HD12	2.55	0.41
1:A:215:TRP:CD1	1:A:221[B]:ILE:HD12	2.55	0.41
1:A:392:TYR:CD1	6:A:1506:78N:H71	2.56	0.41
1:A:80:GLN:NE2	8:A:2004:HOH:O	2.45	0.41
1:B:235:ARG:NH1	1:B:239:GLU:OE2	2.54	0.41
1:A:464:LEU:HB2	2:A:1493:78M:H52C	2.03	0.41
1:B:92:ALA:HB1	2:B:1496:78M:H7	2.02	0.40
1:A:241:VAL:HG11	1:A:290:THR:HG21	2.04	0.40
1:B:56:ARG:NH1	1:B:414:GLY:HA2	2.36	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	427/458 (93%)	413 (97%)	14 (3%)	0	100	100
1	B	439/458 (96%)	423 (96%)	16 (4%)	0	100	100
All	All	866/916 (94%)	836 (96%)	30 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	351/370 (95%)	346 (99%)	5 (1%)	74	88
1	B	362/370 (98%)	358 (99%)	4 (1%)	80	92
All	All	713/740 (96%)	704 (99%)	9 (1%)	76	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ASP
1	A	177	LEU
1	A	291	THR
1	A	295	ASP
1	A	341	GLU
1	B	172	PHE
1	B	214	GLN
1	B	362	ARG
1	B	440	GLN

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 molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 31 ligands modelled in this entry, 5 are monoatomic - leaving 26 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	78M	A	1491	-	10,10,21	1.64	2 (20%)	8,9,22	0.95	1 (12%)
2	78M	A	1492	-	14,14,21	1.38	2 (14%)	13,13,22	0.96	1 (7%)
2	78M	A	1493	-	14,14,21	1.39	2 (14%)	13,13,22	0.93	1 (7%)
2	78M	A	1494	-	10,10,21	1.64	2 (20%)	8,9,22	0.98	1 (12%)
2	78M	A	1495	-	10,10,21	1.64	2 (20%)	8,9,22	0.93	1 (12%)
2	78M	A	1496	-	10,10,21	1.64	2 (20%)	8,9,22	0.98	1 (12%)
2	78M	A	1497	-	7,7,21	1.80	2 (28%)	6,6,22	1.30	1 (16%)
2	78M	A	1498	-	7,7,21	1.27	1 (14%)	6,6,22	1.16	1 (16%)
2	78M	A	1499	-	6,6,21	0.24	0	5,5,22	0.48	0
2	78M	A	1500	-	7,7,21	1.28	1 (14%)	6,6,22	1.16	1 (16%)
2	78M	A	1501	-	7,7,21	1.27	1 (14%)	6,6,22	1.17	1 (16%)
3	LDA	A	1502	-	15,15,15	3.91	2 (13%)	16,17,17	0.60	0
6	78N	A	1506	-	21,21,21	0.94	1 (4%)	22,22,22	0.95	1 (4%)
6	78N	A	1507	-	21,21,21	0.96	1 (4%)	22,22,22	0.98	1 (4%)
7	ACT	A	1508	5	1,3,3	1.16	0	0,3,3	0.00	-
2	78M	B	1491	-	9,9,21	1.73	2 (22%)	8,8,22	1.57	1 (12%)
2	78M	B	1492	-	8,8,21	1.67	2 (25%)	7,7,22	1.07	1 (14%)
2	78M	B	1493	-	13,13,21	1.44	2 (15%)	12,12,22	0.94	1 (8%)
2	78M	B	1494	-	9,9,21	1.69	2 (22%)	8,8,22	1.26	1 (12%)
2	78M	B	1495	-	10,10,21	1.64	2 (20%)	8,9,22	0.96	1 (12%)
2	78M	B	1496	-	10,10,21	1.64	2 (20%)	8,9,22	0.91	1 (12%)
2	78M	B	1497	-	10,10,21	1.64	2 (20%)	8,9,22	0.94	1 (12%)
2	78M	B	1498	-	8,8,21	1.67	2 (25%)	7,7,22	1.07	1 (14%)
2	78M	B	1501	-	21,21,21	0.97	1 (4%)	22,22,22	0.97	1 (4%)
2	78M	B	1502	-	21,21,21	0.97	1 (4%)	22,22,22	0.99	1 (4%)
2	78M	B	1503	-	21,21,21	0.98	1 (4%)	22,22,22	0.99	1 (4%)

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	78M	A	1491	-	-	0/8/8/21	0/0/0/0
2	78M	A	1492	-	-	0/12/12/21	0/0/0/0
2	78M	A	1493	-	-	0/12/12/21	0/0/0/0
2	78M	A	1494	-	-	0/8/8/21	0/0/0/0
2	78M	A	1495	-	-	0/8/8/21	0/0/0/0
2	78M	A	1496	-	-	0/8/8/21	0/0/0/0
2	78M	A	1497	-	-	0/5/5/21	0/0/0/0
2	78M	A	1498	-	-	0/5/5/21	0/0/0/0
2	78M	A	1499	-	-	0/4/4/21	0/0/0/0
2	78M	A	1500	-	-	0/5/5/21	0/0/0/0
2	78M	A	1501	-	-	0/5/5/21	0/0/0/0
3	LDA	A	1502	-	-	0/13/13/13	0/0/0/0
6	78N	A	1506	-	-	0/21/21/21	0/0/0/0
6	78N	A	1507	-	-	0/21/21/21	0/0/0/0
7	ACT	A	1508	5	-	0/0/0/0	0/0/0/0
2	78M	B	1491	-	-	0/7/7/21	0/0/0/0
2	78M	B	1492	-	-	0/6/6/21	0/0/0/0
2	78M	B	1493	-	-	0/11/11/21	0/0/0/0
2	78M	B	1494	-	-	0/7/7/21	0/0/0/0
2	78M	B	1495	-	-	0/8/8/21	0/0/0/0
2	78M	B	1496	-	-	0/8/8/21	0/0/0/0
2	78M	B	1497	-	-	0/8/8/21	0/0/0/0
2	78M	B	1498	-	-	0/6/6/21	0/0/0/0
2	78M	B	1501	-	-	0/21/21/21	0/0/0/0
2	78M	B	1502	-	-	0/21/21/21	0/0/0/0
2	78M	B	1503	-	-	0/21/21/21	0/0/0/0

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1502	LDA	O1-N1	-14.71	1.25	1.39
2	A	1493	78M	C9-C8	-3.79	1.33	1.50
2	A	1494	78M	C9-C8	-3.79	1.33	1.50
2	A	1495	78M	C9-C8	-3.79	1.33	1.50
2	B	1497	78M	C9-C8	-3.79	1.33	1.50
2	A	1491	78M	C9-C8	-3.78	1.33	1.50
2	A	1496	78M	C9-C8	-3.78	1.33	1.50
2	B	1496	78M	C9-C8	-3.78	1.33	1.50
2	B	1493	78M	C9-C8	-3.78	1.33	1.50
2	B	1495	78M	C9-C8	-3.77	1.33	1.50
2	B	1491	78M	C6-C7	-3.77	1.33	1.50
2	A	1492	78M	C9-C8	-3.76	1.33	1.50
2	B	1494	78M	C9-C8	-3.66	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1492	78M	C9-C8	-3.62	1.33	1.49
2	B	1498	78M	C9-C8	-3.59	1.33	1.49
2	A	1497	78M	C5-C4	-3.15	1.33	1.51
3	A	1502	LDA	C1-N1	-3.08	1.45	1.51
2	B	1498	78M	C7-C8	2.95	1.51	1.29
2	B	1492	78M	C7-C8	2.95	1.51	1.29
2	A	1501	78M	C8-C7	3.27	1.51	1.28
2	A	1498	78M	C8-C7	3.28	1.51	1.28
2	A	1500	78M	C8-C7	3.28	1.51	1.28
2	A	1492	78M	C8-C7	3.40	1.51	1.31
2	B	1494	78M	C8-C7	3.41	1.51	1.31
2	B	1496	78M	C8-C7	3.42	1.51	1.31
2	A	1495	78M	C8-C7	3.42	1.51	1.31
2	B	1497	78M	C8-C7	3.42	1.51	1.31
2	A	1494	78M	C8-C7	3.43	1.51	1.31
2	B	1495	78M	C8-C7	3.43	1.51	1.31
2	B	1493	78M	C8-C7	3.43	1.51	1.31
2	A	1491	78M	C8-C7	3.43	1.51	1.31
2	A	1493	78M	C8-C7	3.44	1.51	1.31
2	B	1491	78M	C8-C7	3.44	1.51	1.31
2	A	1496	78M	C8-C7	3.44	1.51	1.31
2	A	1497	78M	C8-C7	3.48	1.52	1.28
6	A	1506	78N	O16-C8	4.08	1.45	1.33
6	A	1507	78N	O16-C8	4.16	1.45	1.33
2	B	1501	78M	O2-C1	4.20	1.46	1.33
2	B	1502	78M	O2-C1	4.23	1.46	1.33
2	B	1503	78M	O2-C1	4.27	1.46	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1491	78M	C9-C8-C7	-3.92	109.14	127.06
2	A	1500	78M	C6-C7-C8	-2.61	109.41	127.08
2	A	1501	78M	C6-C7-C8	-2.60	109.50	127.08
2	A	1498	78M	C6-C7-C8	-2.59	109.53	127.08
2	A	1496	78M	C6-C7-C8	-2.48	108.08	125.34
2	B	1492	78M	C6-C7-C8	-2.48	109.73	133.31
2	B	1498	78M	C6-C7-C8	-2.42	110.30	133.31
2	A	1497	78M	C6-C7-C8	-2.39	110.94	127.08
2	A	1494	78M	C6-C7-C8	-2.38	108.76	125.34
2	B	1496	78M	C6-C7-C8	-2.30	109.30	125.34
2	A	1491	78M	C6-C7-C8	-2.29	109.40	125.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1494	78M	C6-C7-C8	-2.28	109.50	125.34
2	B	1495	78M	C6-C7-C8	-2.24	109.77	125.34
2	A	1495	78M	C6-C7-C8	-2.20	109.99	125.34
2	A	1493	78M	C6-C7-C8	-2.19	110.07	125.34
2	A	1492	78M	C6-C7-C8	-2.19	110.12	125.34
2	B	1493	78M	C6-C7-C8	-2.17	110.22	125.34
2	B	1497	78M	C6-C7-C8	-2.15	110.36	125.34
6	A	1506	78N	O16-C8-C7	2.84	120.54	111.90
2	B	1501	78M	O2-C1-C2	2.84	120.57	111.90
2	B	1502	78M	O2-C1-C2	2.97	120.96	111.90
6	A	1507	78N	O16-C8-C7	3.00	121.05	111.90
2	B	1503	78M	O2-C1-C2	3.07	121.25	111.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1492	78M	1	0
2	A	1493	78M	1	0
2	A	1494	78M	2	0
2	A	1495	78M	1	0
2	A	1496	78M	1	0
2	A	1499	78M	1	0
2	A	1501	78M	1	0
6	A	1506	78N	1	0
2	B	1492	78M	1	0
2	B	1496	78M	2	0
2	B	1498	78M	1	0
2	B	1501	78M	3	0
2	B	1502	78M	3	0
2	B	1503	78M	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 ⓘ

### 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	429/458 (93%)	0.51	36 (8%) 14 13	18, 36, 73, 116	0
1	B	439/458 (95%)	0.56	42 (9%) 10 10	14, 40, 74, 110	0
All	All	868/916 (94%)	0.54	78 (8%) 12 11	14, 38, 74, 116	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	ASN	8.6
1	A	294	ASP	7.1
1	A	117	ASP	6.7
1	A	295	ASP	6.2
1	B	294	ASP	5.4
1	A	236	ARG	5.4
1	A	292	THR	5.1
1	B	232	GLY	5.1
1	B	295	ASP	5.0
1	B	38	ALA	4.9
1	B	296	ARG	4.3
1	B	409	ASP	4.3
1	A	439	LYS	4.3
1	B	176	LEU	4.1
1	B	293	VAL	4.1
1	A	118	GLY	4.0
1	B	338	LYS	3.9
1	B	292	THR	3.9
1	B	336	GLY	3.8
1	A	338	LYS	3.8
1	A	411	GLY	3.7
1	A	299	ALA	3.5
1	B	477	SER	3.4
1	B	298	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	340	GLY	3.3
1	A	291	THR	3.3
1	A	243	ASN	3.2
1	A	413	SER	3.1
1	A	440	GLN	3.1
1	A	200	GLU	3.0
1	B	243	ASN	3.0
1	B	297	ARG	3.0
1	B	322	GLU	2.9
1	B	290	THR	2.9
1	B	339	ASP	2.8
1	B	117	ASP	2.8
1	B	410	ILE	2.7
1	A	298	ILE	2.7
1	A	137	GLY	2.7
1	B	104	LEU	2.6
1	A	293	VAL	2.6
1	A	120	GLU	2.6
1	B	291	THR	2.6
1	A	416	ASN	2.6
1	A	473	PRO	2.6
1	B	476	ASP	2.5
1	B	217	PRO	2.5
1	A	296	ARG	2.5
1	B	267	ARG	2.5
1	B	65	THR	2.5
1	A	195	ASP	2.5
1	B	60	THR	2.5
1	A	248	TYR	2.5
1	A	339	ASP	2.4
1	A	407	ASP	2.4
1	B	413	SER	2.4
1	B	39	PRO	2.3
1	B	420	GLN	2.3
1	A	244	LEU	2.3
1	B	57	ASP	2.3
1	A	81	TRP	2.3
1	A	103	THR	2.2
1	B	105	GLN	2.2
1	B	199	PRO	2.2
1	B	241	VAL	2.2
1	B	240	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	236	ARG	2.2
1	A	301	GLY	2.1
1	A	64	GLY	2.1
1	B	238	GLY	2.1
1	B	411	GLY	2.1
1	A	119	ARG	2.1
1	A	303	GLN	2.1
1	A	80	GLN	2.1
1	B	303	GLN	2.0
1	B	230	ASP	2.0
1	B	337	GLY	2.0
1	A	420	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	78M	A	1493	15/22	0.80	0.27	10.43	43,49,58,58	0
6	78N	A	1507	22/22	0.76	0.32	8.79	55,65,71,72	0
2	78M	B	1492	9/22	0.89	0.32	8.71	39,40,40,41	0
2	78M	B	1496	11/22	0.69	0.39	7.91	43,47,49,49	0
2	78M	A	1499	7/22	0.80	0.27	6.66	46,48,48,49	0
2	78M	B	1497	11/22	0.81	0.26	6.29	51,52,53,53	0
2	78M	A	1497	8/22	0.81	0.23	6.09	47,48,51,52	0
2	78M	A	1500	8/22	0.82	0.24	5.47	44,45,46,47	0
2	78M	B	1493	14/22	0.80	0.33	5.03	48,55,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	78M	B	1495	11/22	0.82	0.27	3.96	44,46,48,49	0
6	78N	A	1506	22/22	0.84	0.22	3.26	37,44,51,52	0
2	78M	B	1502	22/22	0.74	0.33	3.25	48,61,66,68	0
2	78M	A	1494	11/22	0.87	0.23	2.97	35,36,38,39	0
2	78M	B	1498	9/22	0.83	0.24	2.88	47,52,55,55	0
3	LDA	A	1502	16/16	0.70	0.31	2.60	49,58,78,78	0
2	78M	B	1503	22/22	0.72	0.27	2.56	39,48,60,62	0
2	78M	A	1491	11/22	0.89	0.22	2.44	30,36,42,43	0
2	78M	B	1501	22/22	0.75	0.25	2.39	49,55,63,65	0
2	78M	A	1498	8/22	0.85	0.20	1.72	47,49,49,50	0
2	78M	A	1496	11/22	0.84	0.23	0.52	40,41,47,48	0
2	78M	A	1492	15/22	0.84	0.18	0.16	44,46,48,49	0
2	78M	B	1494	10/22	0.88	0.17	-0.30	33,36,41,42	0
2	78M	B	1491	10/22	0.88	0.14	-0.54	38,43,50,51	0
4	MG	A	1503	1/1	0.94	0.09	-1.73	30,30,30,30	0
5	CU	B	1499	1/1	0.59	0.09	-2.31	78,78,78,78	0
5	CU	A	1505	1/1	0.69	0.09	-4.52	77,77,77,77	0
2	78M	A	1501	8/22	0.80	0.19	-	48,49,50,50	0
5	CU	B	1500	1/1	0.86	0.06	-	67,67,67,67	0
5	CU	A	1504	1/1	0.85	0.10	-	62,62,62,62	0
2	78M	A	1495	11/22	0.80	0.21	-	44,46,48,49	0
7	ACT	A	1508	4/4	0.86	0.29	-	55,56,57,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.