



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 7, 2021 – 10:09 AM EDT

PDB ID : 7MJF  
Title : Crystal structure of Candidatus Liberibacter solanacearum dihydrodipicolinate synthase with pyruvate and succinic semi-aldehyde bound in active site  
Authors : Gilkes, J.; Frampton, R.A.; Board, A.J.; Sheen, C.R.; Smith, G.R.; Dobson, R.C.J.  
Deposited on : 2021-04-20  
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.22
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)	:	2.22

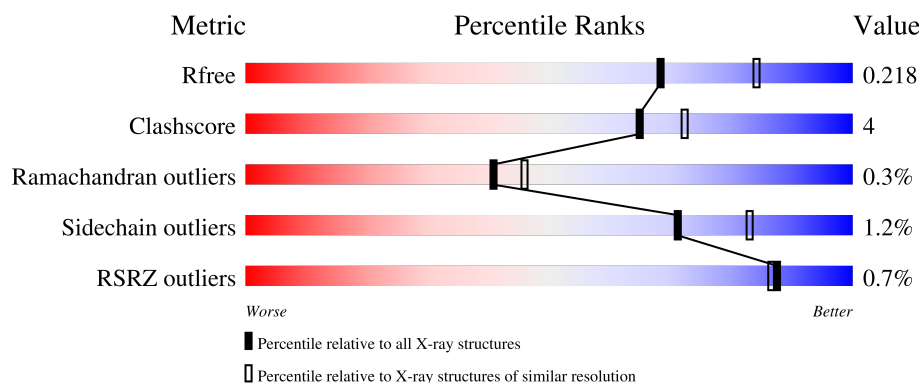
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	296	<div> <div style="width: 94%;"></div> <div style="width: 5%;"></div> </div>
1	B	296	<div> <div style="width: 90%;"></div> <div style="width: 8%;"></div> <div style="width: 2%;"></div> </div>
1	C	296	<div> <div style="width: 88%;"></div> <div style="width: 10%;"></div> <div style="width: 2%;"></div> </div>
1	D	296	<div> <div style="width: 87%;"></div> <div style="width: 12%;"></div> <div style="width: 1%;"></div> </div>
1	E	296	<div> <div style="width: 88%;"></div> <div style="width: 12%;"></div> <div style="width: 1%;"></div> </div>

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Mol	Chain	Length	Quality of chain
1	F	296	<div><div>%</div><div><div></div><div>90%</div><div>10%</div><div></div></div><div></div></div>

## 2 Entry composition [i](#)

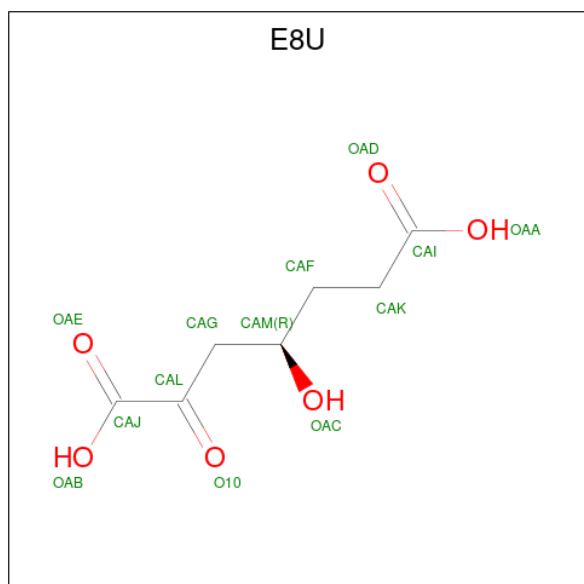
There are 4 unique types of molecules in this entry. The entry contains 14512 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 4-hydroxy-tetrahydrodipicolinate synthase.

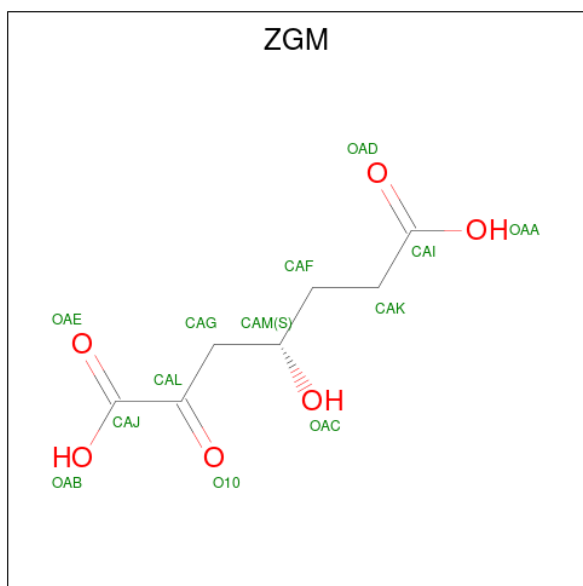
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	2	0
			2251	1418	381	439	13			
1	B	296	Total	C	N	O	S	0	1	0
			2243	1413	380	438	12			
1	C	296	Total	C	N	O	S	0	2	0
			2248	1417	380	438	13			
1	D	296	Total	C	N	O	S	0	1	0
			2243	1413	380	438	12			
1	E	296	Total	C	N	O	S	0	1	0
			2243	1413	380	438	12			
1	F	296	Total	C	N	O	S	0	1	0
			2243	1413	380	438	12			

- Molecule 2 is (4R)-4-oxidanyl-2-oxidanylidene-heptanedioic acid (three-letter code: E8U) (formula: C<sub>7</sub>H<sub>10</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 7 5	0	1
2	B	1	Total C O 12 7 5	0	1
2	C	1	Total C O 12 7 5	0	1
2	D	1	Total C O 12 7 5	0	1
2	E	1	Total C O 12 7 5	0	1
2	F	1	Total C O 12 7 5	0	1

- Molecule 3 is (4S)-4-hydroxy-2-oxoheptanedioic acid (three-letter code: ZGM) (formula:  $C_7H_{10}O_6$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 7 5	0	1
3	B	1	Total C O 12 7 5	0	1
3	C	1	Total C O 12 7 5	0	1
3	D	1	Total C O 12 7 5	0	1
3	E	1	Total C O 12 7 5	0	1

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	1
			12	7	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	246	Total	O	0	0
			246	246		
4	B	222	Total	O	0	0
			222	222		
4	C	123	Total	O	0	0
			123	123		
4	D	124	Total	O	0	0
			124	124		
4	E	89	Total	O	0	0
			89	89		
4	F	93	Total	O	0	0
			93	93		

### 3 Residue-property plots [i](#)

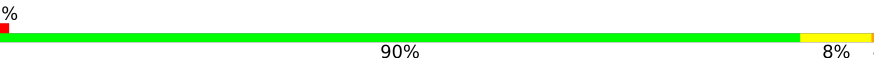
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 4-hydroxy-tetrahydrodipicolinate synthase

Chain A: 




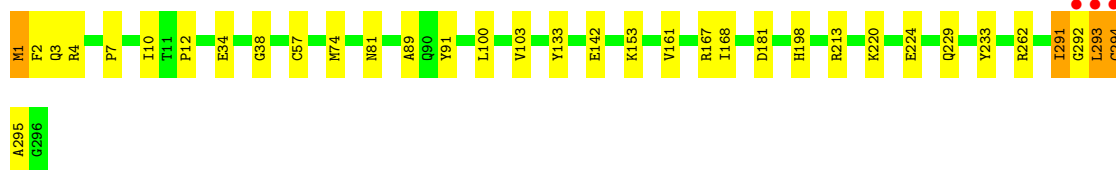
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain B: 




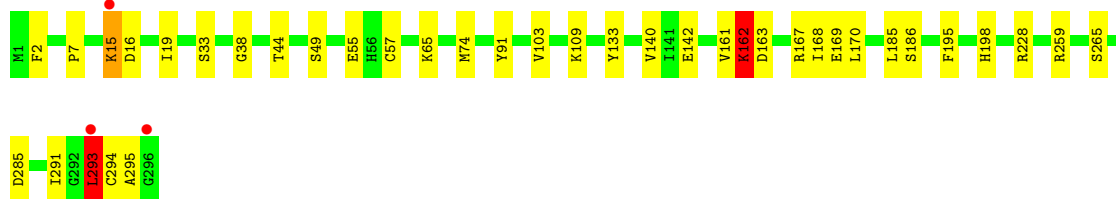
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain C: 




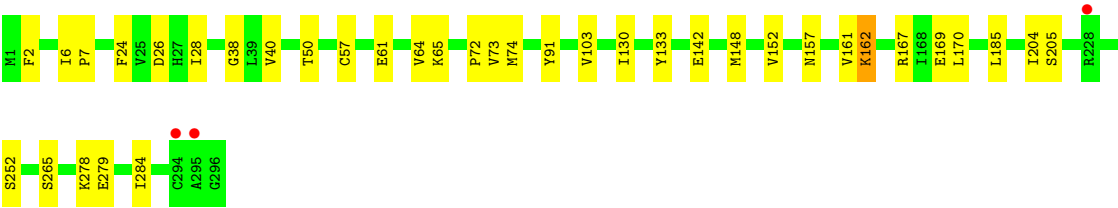
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain D: 

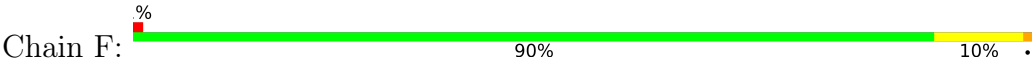


- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain E: 



● Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.10Å 132.88Å 155.06Å 90.00° 99.96° 90.00°	Depositor
Resolution (Å)	45.10 – 2.20 45.88 – 1.92	Depositor EDS
% Data completeness (in resolution range)	96.9 (45.10-2.20) 99.3 (45.88-1.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 1.92Å)	Xtriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, $R_{free}$	0.156 , 0.208 0.173 , 0.218	Depositor DCC
$R_{free}$ test set	7598 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZGM, E8U

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	3/2290 (0.1%)	0.67	2/3106 (0.1%)
1	B	0.65	4/2282 (0.2%)	0.72	5/3096 (0.2%)
1	C	0.40	0/2290	0.61	2/3106 (0.1%)
1	D	0.80	3/2282 (0.1%)	0.77	9/3096 (0.3%)
1	E	0.49	3/2282 (0.1%)	0.63	3/3096 (0.1%)
1	F	0.50	3/2282 (0.1%)	0.65	3/3096 (0.1%)
All	All	0.60	16/13708 (0.1%)	0.68	24/18596 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	1
1	F	0	1
All	All	0	4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	162[A]	LYS	C-N	-20.34	0.87	1.34
1	D	162[B]	LYS	C-N	-20.34	0.87	1.34
1	A	162[A]	LYS	C-N	-15.06	0.99	1.34
1	A	162[B]	LYS	C-N	-15.06	0.99	1.34
1	D	161	VAL	C-N	-15.02	0.99	1.34
1	B	162[A]	LYS	C-N	-13.16	1.03	1.34
1	B	162[B]	LYS	C-N	-13.16	1.03	1.34
1	F	161	VAL	C-N	-11.55	1.07	1.34
1	E	162[A]	LYS	C-N	-9.77	1.11	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	162[B]	LYS	C-N	-9.77	1.11	1.34
1	A	161	VAL	C-N	-9.72	1.11	1.34
1	B	161	VAL	C-N	-9.37	1.12	1.34
1	F	162[A]	LYS	C-N	-8.34	1.14	1.34
1	F	162[B]	LYS	C-N	-8.34	1.14	1.34
1	E	161	VAL	C-N	-7.96	1.15	1.34
1	B	291	ILE	C-N	-5.13	1.23	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	161	VAL	O-C-N	-13.17	101.63	122.70
1	B	161	VAL	C-N-CA	12.99	154.19	121.70
1	D	161	VAL	C-N-CA	12.99	154.17	121.70
1	F	161	VAL	C-N-CA	12.98	154.14	121.70
1	E	161	VAL	C-N-CA	10.82	148.76	121.70
1	D	161	VAL	O-C-N	-10.59	105.76	122.70
1	D	162[A]	LYS	C-N-CA	10.09	146.94	121.70
1	D	162[B]	LYS	C-N-CA	10.09	146.94	121.70
1	A	161	VAL	C-N-CA	9.87	146.38	121.70
1	E	161	VAL	O-C-N	-9.83	106.97	122.70
1	B	161	VAL	O-C-N	-9.08	108.17	122.70
1	F	161	VAL	CA-C-N	8.98	136.95	117.20
1	C	161	VAL	C-N-CA	7.69	140.92	121.70
1	D	161	VAL	CA-C-N	7.52	133.75	117.20
1	D	162[A]	LYS	CA-C-N	6.97	132.53	117.20
1	D	162[B]	LYS	CA-C-N	6.97	132.53	117.20
1	B	162[A]	LYS	O-C-N	6.89	133.72	122.70
1	B	162[B]	LYS	O-C-N	6.89	133.72	122.70
1	E	161	VAL	CA-C-N	6.58	131.66	117.20
1	B	161	VAL	CA-C-N	6.29	131.04	117.20
1	A	161	VAL	O-C-N	-5.65	113.66	122.70
1	D	162[A]	LYS	O-C-N	-5.53	113.85	122.70
1	D	162[B]	LYS	O-C-N	-5.53	113.85	122.70
1	C	291	ILE	C-N-CA	5.26	133.35	122.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	VAL	Mainchain
1	D	162[B]	LYS	Mainchain

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Mol	Chain	Res	Type	Group
1	F	161	VAL	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2251	0	2238	9	0
1	B	2243	0	2227	22	0
1	C	2248	0	2237	24	0
1	D	2243	0	2228	21	0
1	E	2243	0	2228	18	0
1	F	2243	0	2228	21	0
2	A	12	0	8	0	0
2	B	12	0	8	0	0
2	C	12	0	8	0	0
2	D	12	0	8	1	0
2	E	12	0	8	0	0
2	F	12	0	8	0	0
3	A	12	0	0	1	0
3	B	12	0	0	1	0
3	C	12	0	0	0	0
3	D	12	0	0	1	0
3	E	12	0	0	0	0
3	F	12	0	0	0	0
4	A	246	0	0	0	2
4	B	222	0	0	4	1
4	C	123	0	0	1	0
4	D	124	0	0	0	0
4	E	89	0	0	0	0
4	F	93	0	0	0	0
All	All	14512	0	13434	111	2

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 4.

All (111) 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:D:162[A]:LYS:C	1:D:163:ASP:CA	2.27	1.03
1:C:293:LEU:O	1:C:294:CYS:C	2.05	0.93
1:B:291:ILE:O	1:B:293:LEU:N	2.02	0.93
1:B:291:ILE:C	1:B:293:LEU:H	1.73	0.84
1:B:15:LYS:H	1:B:15:LYS:HD2	1.44	0.82
1:D:162[A]:LYS:C	1:D:163:ASP:N	0.87	0.81
1:B:291:ILE:HG13	1:B:293:LEU:HB2	1.67	0.77
1:B:15:LYS:NZ	4:B:401:HOH:O	2.22	0.73
1:B:291:ILE:C	1:B:293:LEU:N	2.45	0.69
1:C:103:VAL:HA	1:C:133:TYR:HB3	1.77	0.67
1:C:142:GLU:OE1	1:C:167:ARG:NH2	2.28	0.66
1:B:295:ALA:HB1	4:B:579:HOH:O	1.97	0.63
1:F:24:PHE:HD2	1:F:62:LEU:HD22	1.65	0.61
1:C:34:GLU:OE2	1:C:213:ARG:NH2	2.33	0.61
1:E:103:VAL:HA	1:E:133:TYR:HB3	1.84	0.60
1:D:103:VAL:HA	1:D:133:TYR:HB3	1.84	0.60
1:F:25:VAL:HG22	1:F:62:LEU:HD21	1.84	0.58
1:C:168:ILE:HD13	1:D:168:ILE:HD13	1.84	0.58
1:E:2:PHE:CZ	1:E:72:PRO:HB2	2.39	0.58
1:C:293:LEU:O	1:C:295:ALA:N	2.36	0.58
1:E:61:GLU:O	1:E:65:LYS:HG2	2.03	0.57
1:D:44:THR:HB	2:D:301[A]:E8U:OAE	2.03	0.57
1:F:103:VAL:HA	1:F:133:TYR:HB3	1.85	0.56
1:D:259:ARG:HD3	1:D:285:ASP:OD1	2.06	0.56
1:C:291:ILE:O	1:C:293:LEU:N	2.39	0.56
1:D:44:THR:HB	3:D:302[B]:ZGM:OAE	2.07	0.55
1:E:57:CYS:HB3	1:E:91:TYR:CE1	2.43	0.54
1:A:168:ILE:HD12	1:A:198:HIS:CD2	2.42	0.54
1:F:149:ALA:O	1:F:153:LYS:HG3	2.07	0.54
1:E:162[B]:LYS:HA	1:E:185:LEU:O	2.07	0.53
1:B:168:ILE:HD12	1:B:198:HIS:CD2	2.44	0.53
1:B:103:VAL:HA	1:B:133:TYR:HB3	1.89	0.53
1:B:19:ILE:HD11	1:B:55:GLU:HB3	1.92	0.52
1:C:220:LYS:NZ	1:C:224:GLU:OE2	2.39	0.52
1:F:56:HIS:O	1:F:60:VAL:HG23	2.11	0.51
1:A:103:VAL:HA	1:A:133:TYR:HB3	1.92	0.51
1:F:194:GLY:O	1:F:197:VAL:HG12	2.11	0.50
1:F:57:CYS:HB3	1:F:91:TYR:CE1	2.46	0.50
1:B:58:ARG:NH1	1:B:61:GLU:OE1	2.43	0.50
1:F:291:ILE:HG22	1:F:293:LEU:HG	1.93	0.50
1:F:21:GLU:O	1:F:25:VAL:HG23	2.12	0.49
1:A:187:GLY:O	3:A:302[B]:ZGM:OAC	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:PRO:HD2	1:F:38:GLY:O	2.13	0.49
1:F:2:PHE:CZ	1:F:72:PRO:HB2	2.47	0.49
1:A:7:PRO:HD2	1:A:38:GLY:O	2.13	0.49
1:A:294:CYS:SG	1:C:295:ALA:HB1	2.53	0.48
1:E:142:GLU:OE1	1:E:167:ARG:NH2	2.44	0.48
1:B:295:ALA:HB3	4:B:420:HOH:O	2.13	0.48
1:E:7:PRO:HD2	1:E:38:GLY:O	2.13	0.48
1:F:1:MET:HE1	1:F:98:ASP:HB3	1.95	0.48
1:D:7:PRO:HD2	1:D:38:GLY:O	2.14	0.47
1:C:229:GLN:OE1	1:C:233:TYR:HE2	1.97	0.47
1:C:291:ILE:C	1:C:293:LEU:N	2.67	0.47
1:D:15:LYS:HD2	1:D:15:LYS:H	1.77	0.47
1:B:187:GLY:O	3:B:302[B]:ZGM:OAC	2.33	0.47
1:C:262:ARG:HE	1:C:262:ARG:HB3	1.52	0.47
1:D:168:ILE:HD12	1:D:198:HIS:CD2	2.50	0.47
1:D:57:CYS:HB3	1:D:91:TYR:CE1	2.50	0.46
1:C:168:ILE:HD12	1:C:198:HIS:CD2	2.50	0.46
1:D:49:SER:HB3	1:F:80:ASN:HD21	1.79	0.46
1:E:169:GLU:HG3	1:E:170:LEU:N	2.30	0.46
1:E:279:GLU:H	1:E:279:GLU:CD	2.19	0.46
1:F:213:ARG:HH11	1:F:213:ARG:HG3	1.81	0.46
1:C:3:GLN:HG3	1:C:4:ARG:HG3	1.98	0.46
1:F:25:VAL:CG2	1:F:62:LEU:HD21	2.45	0.46
1:A:101:LEU:HD11	1:A:133:TYR:HB2	1.96	0.46
1:B:47:GLU:CD	1:B:250:ILE:HD13	2.36	0.46
1:D:109:LYS:HE3	1:D:140:VAL:HG11	1.96	0.46
1:D:142:GLU:OE1	1:D:167:ARG:NH2	2.49	0.46
1:C:1[A]:MET:HG3	4:C:439:HOH:O	2.15	0.45
1:C:57:CYS:HB3	1:C:91:TYR:CE1	2.51	0.45
1:B:194:GLY:O	1:B:197:VAL:HG12	2.16	0.45
1:B:78:GLY:HA3	4:B:533:HOH:O	2.15	0.45
1:B:7:PRO:HD2	1:B:38:GLY:O	2.17	0.45
1:B:113:LYS:HB2	1:B:113:LYS:HE2	1.81	0.44
1:C:291:ILE:C	1:C:293:LEU:H	2.20	0.44
1:F:133:TYR:CD1	1:F:162[A]:LYS:HD3	2.52	0.44
1:B:260:LEU:HD21	1:B:293:LEU:HD23	2.00	0.44
1:C:7:PRO:HD2	1:C:38:GLY:O	2.18	0.44
1:D:19:ILE:HD11	1:D:55:GLU:HB3	1.99	0.44
1:E:252:SER:HB3	1:E:284:ILE:HD11	1.98	0.44
1:E:148:MET:O	1:E:152:VAL:HG23	2.17	0.44
1:D:169:GLU:HG3	1:D:170:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:LYS:HB2	1:E:278:LYS:NZ	2.29	0.43
1:C:293:LEU:O	1:C:294:CYS:O	2.35	0.43
1:D:291:ILE:CD1	1:D:293:LEU:HD22	2.48	0.43
1:F:133:TYR:CD1	1:F:162[B]:LYS:HD3	2.53	0.43
1:F:37:SER:O	1:F:72:PRO:HD2	2.18	0.43
1:C:181:ASP:N	1:C:181:ASP:OD1	2.52	0.43
1:A:66:THR:O	1:A:70:ARG:NH2	2.42	0.43
1:D:16:ASP:OD1	1:D:16:ASP:N	2.52	0.42
1:F:128:LEU:HD23	1:F:128:LEU:HA	1.86	0.42
1:F:79:SER:HB3	1:F:85:SER:OG	2.20	0.42
1:F:220:LYS:HB3	1:F:220:LYS:HE2	1.72	0.42
1:C:2:PHE:CZ	1:C:74:MET:HB2	2.55	0.42
1:A:2:PHE:CZ	1:A:72:PRO:HB2	2.55	0.42
1:B:7:PRO:HG3	1:B:31:GLN:OE1	2.20	0.42
1:B:101:LEU:HD11	1:B:133:TYR:HB2	2.01	0.42
1:E:24:PHE:O	1:E:28:ILE:HG13	2.19	0.42
1:C:10:ILE:HD12	1:C:12:PRO:HD3	2.01	0.41
1:A:128:LEU:HA	1:A:128:LEU:HD23	1.83	0.41
1:C:81:ASN:ND2	1:E:50:THR:HA	2.35	0.41
1:D:186:SER:HB2	1:D:195:PHE:CG	2.56	0.41
1:E:6:ILE:O	1:E:204:ILE:HA	2.20	0.41
1:C:89:ALA:HB1	1:C:100:LEU:HD13	2.02	0.40
1:E:40:VAL:HG22	1:E:74:MET:HB3	2.03	0.40
1:B:292:GLY:O	1:B:293:LEU:C	2.59	0.40
1:D:2:PHE:CZ	1:D:74:MET:HB2	2.56	0.40
1:D:162[B]:LYS:HA	1:D:185:LEU:O	2.21	0.40
1:E:64:VAL:HG22	1:E:73:VAL:HG11	2.04	0.40
1:E:130:ILE:N	1:E:157:ASN:O	2.49	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:600:HOH:O	4:B:592:HOH:O[4_546]	0.50	1.70
4:A:469:HOH:O	4:A:593:HOH:O[2_656]	0.57	1.63

## 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	295/296 (100%)	288 (98%)	7 (2%)	0	100	100
1	B	295/296 (100%)	288 (98%)	5 (2%)	2 (1%)	22	22
1	C	295/296 (100%)	288 (98%)	5 (2%)	2 (1%)	22	22
1	D	295/296 (100%)	285 (97%)	8 (3%)	2 (1%)	22	22
1	E	295/296 (100%)	289 (98%)	6 (2%)	0	100	100
1	F	295/296 (100%)	290 (98%)	5 (2%)	0	100	100
All	All	1770/1776 (100%)	1728 (98%)	36 (2%)	6 (0%)	41	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	292	GLY
1	B	292	GLY
1	B	293	LEU
1	D	293	LEU
1	C	294	CYS
1	D	295	ALA

### 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	246/244 (101%)	245 (100%)	1 (0%)	91	96
1	B	245/244 (100%)	242 (99%)	3 (1%)	71	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	246/244 (101%)	242 (98%)	4 (2%)	62	76
1	D	245/244 (100%)	238 (97%)	7 (3%)	42	54
1	E	245/244 (100%)	242 (99%)	3 (1%)	71	83
1	F	245/244 (100%)	245 (100%)	0	100	100
All	All	1472/1464 (100%)	1454 (99%)	18 (1%)	71	83

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	ARG
1	B	15	LYS
1	B	265	SER
1	B	294	CYS
1	C	1[A]	MET
1	C	1[B]	MET
1	C	153	LYS
1	C	293	LEU
1	D	15	LYS
1	D	33	SER
1	D	65	LYS
1	D	228	ARG
1	D	265	SER
1	D	293	LEU
1	D	294	CYS
1	E	26	ASP
1	E	205	SER
1	E	265	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	229	GLN
1	E	263	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

12 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	$\# Z  > 2$
3	ZGM	E	302[B]	1	5,11,12	0.36	0	7,13,15	1.65	1 (14%)
3	ZGM	D	302[B]	1	5,11,12	0.46	0	7,13,15	2.48	2 (28%)
3	ZGM	B	302[B]	1	5,11,12	0.37	0	7,13,15	3.14	2 (28%)
2	E8U	B	301[A]	1	5,11,12	0.24	0	7,13,15	2.88	2 (28%)
3	ZGM	C	302[B]	1	5,11,12	0.45	0	7,13,15	3.20	2 (28%)
2	E8U	C	301[A]	1	5,11,12	0.67	0	7,13,15	3.03	1 (14%)
2	E8U	A	301[A]	1	5,11,12	0.62	0	7,13,15	2.75	2 (28%)
2	E8U	E	301[A]	1	5,11,12	0.45	0	7,13,15	1.64	1 (14%)
3	ZGM	F	301[A]	1	5,11,12	0.43	0	7,13,15	1.75	2 (28%)
2	E8U	F	302[B]	1	5,11,12	0.36	0	7,13,15	1.90	1 (14%)
2	E8U	D	301[A]	1	5,11,12	0.50	0	7,13,15	1.92	1 (14%)
3	ZGM	A	302[B]	1	5,11,12	0.71	0	7,13,15	4.62	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ZGM	E	302[B]	1	-	3/6/10/13	-
3	ZGM	D	302[B]	1	-	4/6/10/13	-
3	ZGM	B	302[B]	1	-	6/6/10/13	-
2	E8U	B	301[A]	1	-	1/6/10/13	-
3	ZGM	C	302[B]	1	-	6/6/10/13	-
2	E8U	C	301[A]	1	-	1/6/10/13	-
2	E8U	A	301[A]	1	-	1/6/10/13	-
2	E8U	E	301[A]	1	-	3/6/10/13	-
3	ZGM	F	301[A]	1	-	3/6/10/13	-
2	E8U	F	302[B]	1	-	2/6/10/13	-
2	E8U	D	301[A]	1	-	2/6/10/13	-
3	ZGM	A	302[B]	1	-	6/6/10/13	-

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302[B]	ZGM	CAL-CAG-CAM	-10.84	94.20	115.05
2	C	301[A]	E8U	CAK-CAF-CAM	-7.39	100.83	115.05
3	B	302[B]	ZGM	CAL-CAG-CAM	-7.21	101.17	115.05
2	B	301[A]	E8U	CAK-CAF-CAM	-7.10	101.40	115.05
3	C	302[B]	ZGM	CAL-CAG-CAM	-6.99	101.61	115.05
2	A	301[A]	E8U	CAK-CAF-CAM	-6.19	103.14	115.05
3	A	302[B]	ZGM	CAK-CAF-CAM	-5.09	105.26	115.05
3	D	302[B]	ZGM	CAL-CAG-CAM	-4.79	105.84	115.05
2	D	301[A]	E8U	CAK-CAF-CAM	-4.50	106.39	115.05
2	F	302[B]	E8U	CAK-CAF-CAM	-4.41	106.57	115.05
3	D	302[B]	ZGM	CAK-CAF-CAM	-4.02	107.32	115.05
3	C	302[B]	ZGM	CAK-CAF-CAM	-3.95	107.45	115.05
2	E	301[A]	E8U	CAK-CAF-CAM	-3.78	107.78	115.05
3	B	302[B]	ZGM	CAK-CAF-CAM	-3.21	108.87	115.05
3	F	301[A]	ZGM	CAL-CAG-CAM	-3.13	109.04	115.05
3	E	302[B]	ZGM	CAL-CAG-CAM	-2.92	109.43	115.05
3	F	301[A]	ZGM	CAK-CAF-CAM	-2.42	110.40	115.05
2	A	301[A]	E8U	CAF-CAK-CAI	2.36	118.67	113.59
2	B	301[A]	E8U	CAG-CAL-CAJ	2.22	118.36	113.59

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	301[A]	E8U	CAL-CAG-CAM-CAF
3	A	302[B]	ZGM	CAL-CAG-CAM-CAF
3	A	302[B]	ZGM	CAM-CAF-CAK-CAI
3	B	302[B]	ZGM	CAL-CAG-CAM-CAF
3	C	302[B]	ZGM	CAM-CAF-CAK-CAI
3	D	302[B]	ZGM	CAM-CAG-CAL-CAJ
3	E	302[B]	ZGM	CAM-CAG-CAL-CAJ
3	F	301[A]	ZGM	CAM-CAF-CAK-CAI
3	A	302[B]	ZGM	CAK-CAF-CAM-OAC
3	A	302[B]	ZGM	CAL-CAG-CAM-OAC
3	B	302[B]	ZGM	CAL-CAG-CAM-OAC
3	C	302[B]	ZGM	CAK-CAF-CAM-OAC
3	C	302[B]	ZGM	CAL-CAG-CAM-OAC
2	A	301[A]	E8U	CAM-CAG-CAL-CAJ
2	D	301[A]	E8U	CAM-CAG-CAL-CAJ
3	B	302[B]	ZGM	CAM-CAF-CAK-CAI
2	E	301[A]	E8U	CAL-CAG-CAM-OAC
3	B	302[B]	ZGM	CAK-CAF-CAM-OAC
3	C	302[B]	ZGM	CAL-CAG-CAM-CAF
3	D	302[B]	ZGM	CAL-CAG-CAM-OAC
3	F	301[A]	ZGM	CAK-CAF-CAM-OAC
3	B	302[B]	ZGM	CAK-CAF-CAM-CAG
3	D	302[B]	ZGM	CAL-CAG-CAM-CAF
2	B	301[A]	E8U	CAM-CAG-CAL-CAJ
2	C	301[A]	E8U	CAM-CAG-CAL-CAJ
2	E	301[A]	E8U	CAM-CAG-CAL-CAJ
2	F	302[B]	E8U	CAM-CAF-CAK-CAI
3	A	302[B]	ZGM	CAM-CAG-CAL-CAJ
3	F	301[A]	ZGM	CAM-CAG-CAL-CAJ
2	D	301[A]	E8U	CAK-CAF-CAM-OAC
3	A	302[B]	ZGM	CAK-CAF-CAM-CAG
3	C	302[B]	ZGM	CAK-CAF-CAM-CAG
2	F	302[B]	E8U	CAM-CAG-CAL-CAJ
3	C	302[B]	ZGM	CAM-CAG-CAL-CAJ
3	D	302[B]	ZGM	CAM-CAF-CAK-CAI
3	E	302[B]	ZGM	CAK-CAF-CAM-OAC
3	B	302[B]	ZGM	CAM-CAG-CAL-CAJ
3	E	302[B]	ZGM	CAM-CAF-CAK-CAI

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302[B]	ZGM	1	0
3	B	302[B]	ZGM	1	0
2	D	301[A]	E8U	1	0
3	A	302[B]	ZGM	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	4
1	F	4
1	B	4
1	A	4
1	D	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	161:VAL	C	162[B]:LYS	N	1.17
1	E	161:VAL	C	162[A]:LYS	N	1.15
1	F	162[A]:LYS	C	163:ASP	N	1.14
1	B	161:VAL	C	162[B]:LYS	N	1.13
1	B	161:VAL	C	162[A]:LYS	N	1.12
1	A	161:VAL	C	162[A]:LYS	N	1.11
1	E	162[A]:LYS	C	163:ASP	N	1.11
1	F	161:VAL	C	162[B]:LYS	N	1.11
1	F	162[B]:LYS	C	163:ASP	N	1.11
1	A	161:VAL	C	162[B]:LYS	N	1.10
1	E	162[B]:LYS	C	163:ASP	N	1.08
1	F	161:VAL	C	162[A]:LYS	N	1.07
1	B	162[B]:LYS	C	163:ASP	N	1.04
1	B	162[A]:LYS	C	163:ASP	N	1.03
1	A	162[A]:LYS	C	163:ASP	N	0.99
1	D	161:VAL	C	162[A]:LYS	N	0.99
1	D	161:VAL	C	162[B]:LYS	N	0.98
1	D	162[B]:LYS	C	163:ASP	N	0.92
1	A	162[B]:LYS	C	163:ASP	N	0.91

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	162[A]:LYS	C	163:ASP	N	0.87

## 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, 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	296/296 (100%)	-0.77	0 100 100	23, 32, 49, 76	0
1	B	296/296 (100%)	-0.65	2 (0%) 87 86	24, 33, 52, 116	0
1	C	296/296 (100%)	-0.68	3 (1%) 82 81	36, 45, 64, 118	0
1	D	296/296 (100%)	-0.64	3 (1%) 82 81	33, 46, 66, 138	0
1	E	296/296 (100%)	-0.58	3 (1%) 82 81	38, 54, 75, 94	0
1	F	296/296 (100%)	-0.54	2 (0%) 87 86	35, 52, 74, 94	0
All	All	1776/1776 (100%)	-0.64	13 (0%) 87 86	23, 45, 70, 138	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	292	GLY	8.4
1	D	293	LEU	8.3
1	F	295	ALA	4.6
1	B	294	CYS	4.4
1	C	294	CYS	4.2
1	B	293	LEU	3.2
1	C	293	LEU	2.9
1	D	296	GLY	2.6
1	E	295	ALA	2.4
1	E	228	ARG	2.4
1	F	227	TYR	2.4
1	D	15	LYS	2.1
1	E	294	CYS	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 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	E8U	A	301[A]	12/13	0.87	0.17	27,35,45,48	12
3	ZGM	A	302[B]	12/13	0.88	0.18	27,35,45,48	12
3	ZGM	F	301[A]	12/13	0.89	0.17	59,64,79,88	12
3	ZGM	E	302[B]	12/13	0.90	0.13	55,67,81,81	12
3	ZGM	B	302[B]	12/13	0.90	0.17	34,41,58,68	12
3	ZGM	D	302[B]	12/13	0.91	0.13	48,55,63,64	12
2	E8U	B	301[A]	12/13	0.91	0.17	34,41,58,68	12
2	E8U	E	301[A]	12/13	0.91	0.14	55,67,81,81	12
2	E8U	D	301[A]	12/13	0.92	0.13	48,55,63,64	12
2	E8U	C	301[A]	12/13	0.92	0.11	40,48,57,69	12
3	ZGM	C	302[B]	12/13	0.92	0.11	40,48,57,69	12
2	E8U	F	302[B]	12/13	0.93	0.15	59,64,79,88	12

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

There are no such residues in this entry.